

# CONIC DISPERSION SURFACES FOR POINT SCATTERERS ON A HONEYCOMB LATTICE

MINJAE LEE

**ABSTRACT.** We investigate the spectrum and dispersion relation of Schrödinger operator with point scatterers on a triangular lattice and a honeycomb lattice, respectively. We prove that the low-level dispersion surfaces have conic singularities near Dirac points, which are the vertices of the first Brillouin Zone. The existence of such conic dispersion surface plays an important role in various electronic properties of honeycomb-structured materials such as graphene. We then prove that for the honeycomb lattice, the band spectra generated by higher-level dispersion surfaces are all connected so the complete spectrum consists of at most three bands. Numerical simulations for dispersion surfaces with various coupling constant are also presented.

## 1. INTRODUCTION

In this paper we investigate the spectral properties of the Schrödinger operator with point scatterers, or  $\delta$ -potentials, on the triangular lattice  $\Lambda \subset \mathbb{R}^2$  and honeycomb lattice  $H \subset \mathbb{R}^2$  (See Figure 1). The notion of point scatterers started with the Kronig-Penny model [11] which describes the dispersion relation, or energy-momentum relation, and the band structure of an electron on a 1-dimensional solid crystal. This idea has been generalized to infinitely many point scatterers on a periodic structure in  $\mathbb{R}^d$ ,  $d = 1, 2, 3$  [2] using Krein's theory of self-adjoint extensions. In particular, such a point scatterer can be decomposed into "fibers" [9] parametrized by  $\mathbf{k}$  in  $\mathcal{B}$ , the first Brillouin Zone, which corresponds to the Floquet-Bloch theory [10] for a Schrödinger operator  $-\Delta + V$  where  $V \in C^\infty$  is a periodic potential.

On the other hand, the honeycomb lattices and the periodic potentials with such symmetry structure have drawn considerable interest in the physics community due to the groundbreaking experiment [13] on fabrication technique regarding graphene, a two-dimensional single layer of carbon atoms arranged in the honeycomb lattice structure. Well before then in 1947, using the tight-binding model, P.R. Wallace [12] found that the dispersion surfaces of graphene have conic singularities at Dirac points, the six corners of the First Brillouin Zone. In fact, the wave packet whose momentum components are concentrated near these Dirac points behaves as a solution of two-dimensional Dirac wave equation, which describes the evolution of massless relativistic fermions. In addition, C. Fefferman and M. Weinstein [1] recently showed the existence of conic singularities near Dirac points on the low level dispersion surfaces regardless of the magnitude of the potential.

In the present paper, we first investigate the spectral properties of point scatterers on a triangular lattice, which are similar but simpler compared to that on a honeycomb lattice. The global behavior of the dispersion surfaces and spectral

bands are studied for both the triangular and honeycomb lattices varying the coupling constant  $\alpha$ . For the triangular lattice point scatterers, we observe at most two spectral bands generated by the first dispersion surface and the others, respectively, for some  $\alpha$ . On the other hand, the honeycomb lattice point scatterers produce at most three dispersion surfaces where each band consists of  $j$ -th dispersion surfaces where  $j = 1, 2$ ;  $j = 3$  and  $j \geq 4$ , respectively.

We also prove that near Dirac points the triangular lattice produces conic singularities independent of  $\alpha$  whereas the honeycomb lattice generates conic singularities depending on  $\alpha$ . These results are illustrated numerically by various figures and movies. For the triangular lattice model, see 4, 5, 6 and <http://math.berkeley.edu/~lmj0425/floq1dual.avi>. For the honeycomb lattice model, see 8, 10, 11 and <http://math.berkeley.edu/~lmj0425/floq2dual.avi>.

## 2. LATTICE STRUCTURE ON A 2-DIMENSIONAL SPACE

Let  $\mathbf{v}_1 = a \left( \frac{\sqrt{3}}{2}, \frac{1}{2} \right)$  and  $\mathbf{v}_2 = a \left( \frac{\sqrt{3}}{2}, -\frac{1}{2} \right)$  with  $a > 0$ . Then  $\Lambda = \mathbb{Z}\mathbf{v}_1 \oplus \mathbb{Z}\mathbf{v}_2$  is a triangular lattice with the fundamental domain  $\Gamma = \mathbb{R}^2/\Lambda$ . Note that the fundamental domain  $\Gamma$  contains only one lattice point at  $\mathbf{x} = \mathbf{0}$ .

On the other hand, the union of two triangular lattices generates a honeycomb lattice  $H$ :  $H = \Lambda \cup (\Lambda + \mathbf{x}_0)$  where  $\mathbf{x}_0 = \frac{2}{3}(\mathbf{v}_1 + \mathbf{v}_2)$ . Note that  $\Gamma$  contains two points of  $H$  at  $\mathbf{x} = \mathbf{0}$  and  $\mathbf{x} = \mathbf{x}_0$ .

The dual lattice  $\Lambda^* = \mathbb{Z}\mathbf{k}_1 \oplus \mathbb{Z}\mathbf{k}_2$  is spanned by two vectors  $\mathbf{k}_1, \mathbf{k}_2$  satisfying

$$\mathbf{k}_i \cdot \mathbf{v}_j = 2\pi\delta_{ij}, \quad i, j = 1, 2$$

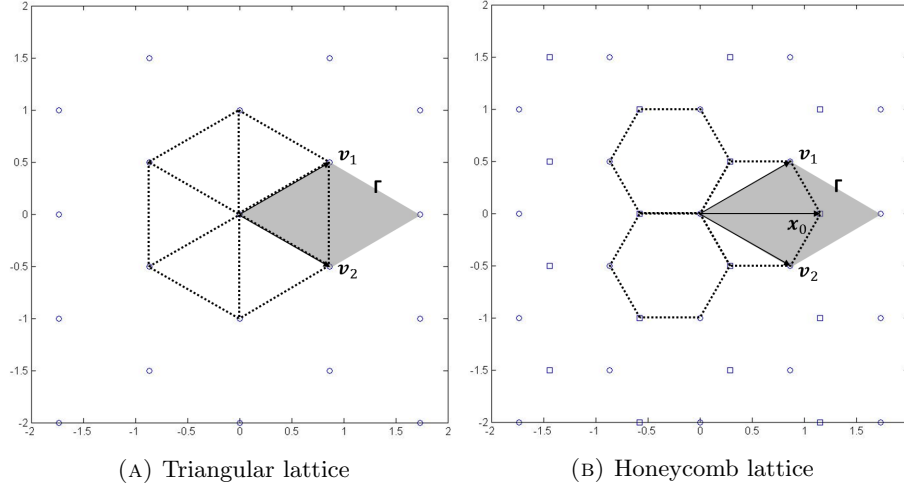


FIGURE 1. Two kind of lattice structures generated by two vectors  $\mathbf{v}_1 = \left( \frac{\sqrt{3}}{2}, \frac{1}{2} \right)$  and  $\mathbf{v}_2 = \left( \frac{\sqrt{3}}{2}, -\frac{1}{2} \right)$ .  $\Gamma$  is the fundamental domain of the lattice. The translated triangular lattice points on the honeycomb lattice are marked as  $\square$ .

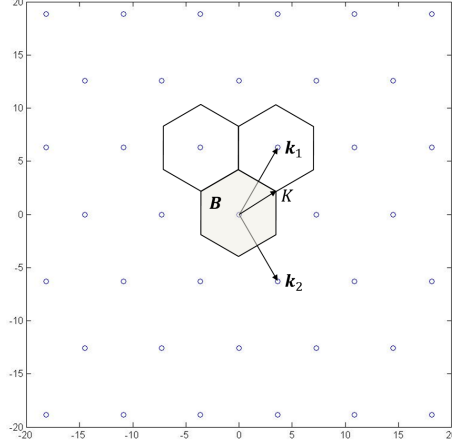


FIGURE 2. The dual of the triangular lattice  $\Lambda$  with Brillouin Zone  $\mathcal{B}$  and a Dirac point  $\mathbf{K}$

or equivalently,

$$\mathbf{k}_1 = \frac{4\pi}{a\sqrt{3}} \left( \frac{1}{2}, \frac{\sqrt{3}}{2} \right), \quad \mathbf{k}_2 = \frac{4\pi}{a\sqrt{3}} \left( \frac{1}{2}, -\frac{\sqrt{3}}{2} \right),$$

The Brillouin Zone  $\mathcal{B}$  is defined as a hexagon centered at the origin. (See Figure 2.)

### 3. INTRODUCTION TO POINT SCATTERERS

In this section, we first introduce Floquet theory for smooth periodic potentials. Then we rigorously define the point scatterers on  $\mathbb{R}^2$  using renormalization and the theory of self-adjoint extensions. Then we investigate the corresponding result for point scatterers on a periodic structure.

#### 3.1. Notations.

- (1)  $\mathbf{k}$  is a vector in Brillouin Zone  $\mathcal{B}$
- (2)  $\mathbf{v}_{\mathbf{m}} = \mathbf{v}_{(m_1, m_2)} = m_1 \mathbf{v}_1 + m_2 \mathbf{v}_2$  is a vector in the triangular lattice  $\Lambda$ .
- (3)  $\xi_{\mathbf{m}} = \xi_{(m_1, m_2)} = m_1 \mathbf{k}_1 + m_2 \mathbf{k}_2$  is a vector in the dual lattice  $\Lambda^*$ .
- (4)  $L_{\mathbf{k}}^2(\mathbb{R}^2) = \{f \in L^2(\mathbb{R}^2) \mid f(\mathbf{x} + \mathbf{v}_j) = e^{i\mathbf{k} \cdot \mathbf{v}_j} f(\mathbf{x}), \quad j = 1, 2\}$
- (5)  $H_{\mathbf{k}}^2(\mathbb{R}^2) = \{f \in H^2(\mathbb{R}^2) \mid f(\mathbf{x} + \mathbf{v}_j) = e^{i\mathbf{k} \cdot \mathbf{v}_j} f(\mathbf{x}), \quad j = 1, 2\}$
- (6)  $\Delta(\mathbf{k}) = \Delta$  with Floquet boundary condition:  $D(\Delta(\mathbf{k})) = H_{\mathbf{k}}^2(\mathbb{R}^2)$
- (7)  $(f, g) = \int_{\Gamma} \overline{f(\mathbf{x})} g(\mathbf{x}) d\mathbf{x}, \quad f, g \in L^2(\Gamma)$
- (8)  $\text{mult}(\lambda, P)$  is the multiplicity of the eigenvalue  $\lambda$  with the operator  $P$ .

**3.2. Floquet Theory.** Suppose  $V$  is smooth and periodic. Then we can expand  $V$  in a Fourier series:

$$V(\mathbf{x}) = \sum_{\mathbf{m} \in \mathbb{Z}^2} V_{\mathbf{m}} e^{i\xi_{\mathbf{m}} \cdot \mathbf{x}}$$

with the Fourier coefficients

$$V_{\mathbf{m}} = \frac{1}{|\Gamma|} \int_{\Gamma} V(\mathbf{x}) e^{-i\xi_{\mathbf{m}} \cdot \mathbf{x}} d\mathbf{x}$$

Consider a Fourier transform of  $P = -\Delta + V$ . Then

$$(3.1) \quad \hat{P}f(\xi) = \mathcal{F}P\mathcal{F}^{-1}f(\xi) = |\xi|^2 \hat{f}(\xi) + \frac{1}{2\pi} \int_{\mathbb{R}^d} \hat{V}(\xi - \eta) \hat{f}(\eta) d\eta$$

By the Fourier inversion formula, we formally obtain

$$(3.2) \quad \hat{V}(\xi) = 2\pi \sum_{\mathbf{m} \in \mathbb{Z}^2} V_{\mathbf{m}} \delta(\xi - \xi_{\mathbf{m}})$$

since

$$\begin{aligned} V(\mathbf{x}) &= \sum_{\mathbf{m} \in \mathbb{Z}^2} V_{\mathbf{m}} e^{i\xi_{\mathbf{m}} \cdot \mathbf{x}} \\ &= \sum_{\mathbf{m} \in \mathbb{Z}^2} V_{\mathbf{m}} \int_{\mathbb{R}^3} \delta(\xi - \xi_{\mathbf{m}}) e^{i\xi \cdot \mathbf{x}} d\xi \\ &= \frac{1}{2\pi} \int_{\mathbb{R}^3} \hat{V}(\xi) e^{i\xi \cdot \mathbf{x}} \end{aligned}$$

Combining (3.1) and (3.2), we obtain

$$(3.3) \quad \hat{P}\hat{f}(\xi) = |\xi|^2 \hat{f}(\xi) + \sum_{\mathbf{m} \in \mathbb{Z}^2} V_{\mathbf{m}} \hat{f}(\xi - \xi_{\mathbf{m}})$$

Hence the eigenvalue problem  $(P - \lambda)f = 0$ ,  $\lambda \in \mathbb{R}$  becomes an algebraic problem

$$(3.4) \quad (|\xi|^2 - \lambda) \hat{f}(\xi) + \sum_{\mathbf{m} \in \mathbb{Z}^2} V_{\mathbf{m}} \hat{f}(\xi - \xi_{\mathbf{m}}) = 0, \quad \lambda \in \mathbb{R}$$

which is called the “central equation” [10] for Floquet-Bloch theory.

Now consider a decomposition operator  $\mathcal{U} : L^2(\mathbb{R}^2) \rightarrow \int_{\mathcal{B}}^{\oplus} d\mathbf{k} \, l^2(\Lambda^*)$  defined as

$$\mathcal{U}\hat{f}(\mathbf{k}, \xi_{\mathbf{m}}) = \hat{f}(\xi_{\mathbf{m}} + \mathbf{k}), \quad \hat{f} \in L^2(\mathbb{R}^2)$$

which is equivalent to the simple decomposition of a vector  $\xi \in \mathbb{R}^2$  into a lattice point  $\xi_{\mathbf{m}} \in \Lambda^*$  and the remainder  $\mathbf{k} \in \mathcal{B}$ , i.e.,

$$\xi = \xi_{\mathbf{m}} + \mathbf{k}$$

Then we obtain

$$(3.5) \quad \left( \mathcal{U}^{-1} \hat{P} \mathcal{U} \hat{f} \right) (\mathbf{k}, \xi_{\mathbf{m}}) = \left( \hat{P}(\mathbf{k}) \hat{f}(\mathbf{k}, \bullet) \right) (\xi_{\mathbf{m}})$$

with  $\hat{P}(\mathbf{k}) : l^2(\Lambda^*) \rightarrow l^2(\Lambda^*)$  defined for each  $\mathbf{k} \in \mathcal{B}$  by

$$(3.6) \quad \hat{P}(\mathbf{k})g(\xi_{\mathbf{m}}) = |\xi_{\mathbf{m}} + \mathbf{k}|^2 g(\xi_{\mathbf{m}}) + \sum_{\mathbf{m}' \in \mathbb{Z}^2} V_{\mathbf{m}'} g(\xi_{\mathbf{m}} - \xi_{\mathbf{m}'})$$

Note that (3.5) can also be written

$$(3.7) \quad \mathcal{U}^{-1} \hat{P} \mathcal{U} = \int_{\mathcal{B}}^{\oplus} d\mathbf{k} \hat{P}(\mathbf{k})$$

In addition, we obtain an equivalent result in  $\mathbf{x}$ -space. Define  $P(\mathbf{k}) : L_{\mathbf{k}}^2(\Gamma) \rightarrow L_{\mathbf{k}}^2(\Gamma)$  as the inverse Fourier transform of the operator  $\hat{P}$ , namely,

$$P(\mathbf{k}) = \mathcal{F}^{-1} \hat{P}(\mathbf{k}) \mathcal{F} = -\Delta(\mathbf{k}) + V$$

In particular, if  $V \equiv 0$ , we observe from (3.6) that the spectrum of the free decomposed Hamiltonian  $-\hat{\Delta}(\mathbf{k})$  is discrete. More precisely,

$$\sigma(-\Delta(\mathbf{k})) = \sigma_d(-\Delta(\mathbf{k})) = \{|\xi_{\mathbf{m}} + \mathbf{k}|^2 \mid \mathbf{m} \in \mathbb{Z}^2\}$$

Similarly, the non-zero potentials also produce discrete spectra determined by (3.6). Then we observe

$$\sigma(P) = \sigma(\hat{P}) = \bigcup_{\mathbf{k} \in \mathcal{B}} \sigma(\hat{P}(\mathbf{k})) = \bigcup_{\mathbf{k} \in \mathcal{B}} \sigma(P(\mathbf{k}))$$

Hence, the spectrum of  $P$  appears as a union of bands, each of which consists of one eigenvalue of  $P(\mathbf{k})$  if the dependence in  $\mathbf{k}$  is continuous.

**3.3. Point scatterers on periodic structures.** In this section, we define the one point scatterer, finitely many point scatterers and point scatterers on a periodic structure using self-adjoint extension theory and renormalization process.

**3.3.1. The one point scatterer.** We start with  $P = -\Delta - c\delta$ , a formal Schrödinger operator on  $\mathbb{R}^2$  with a single delta potential at the origin. Expanding the resolvent, we obtain

$$(P - \lambda)^{-1} = (-\Delta - c\delta - \lambda)^{-1} = (1 - cG_\lambda\delta)^{-1}G_\lambda = G_\lambda + \sum_{j=1}^{\infty} (cG_\lambda\delta)^j G_\lambda$$

Then we obtain the integral kernel

$$\begin{aligned} (P - \lambda)^{-1}(\mathbf{x}, \mathbf{x}') &= G_\lambda(\mathbf{x} - \mathbf{x}') - cG_\lambda(\mathbf{x}) \left[ \sum_{j=1}^{\infty} (cG_\lambda(\mathbf{0}))^j \right] G_\lambda(\mathbf{x}') \\ &= G_\lambda(\mathbf{x} - \mathbf{x}') - cG_\lambda(\mathbf{x}) [1 - cG_\lambda(\mathbf{0})]^{-1} G_\lambda(\mathbf{x}') \\ &= G_\lambda(\mathbf{x} - \mathbf{x}') - G_\lambda(\mathbf{x}) [c^{-1} - G_\lambda(\mathbf{0})]^{-1} G_\lambda(\mathbf{x}') \end{aligned}$$

where the integral kernel  $G_\lambda = (-\Delta - \lambda)^{-1}$  of the free resolvent in  $L^2(\mathbb{R}^2)$  reads

$$(3.8) \quad G_\lambda(\mathbf{x}) = \begin{cases} \frac{i}{4} H_0^{(1)}(\sqrt{\lambda}|\mathbf{x}|) & \text{Im } \sqrt{\lambda} > 0, \mathbf{x} \neq \mathbf{0} \\ -\frac{\ln |\mathbf{x}|}{2\pi} & \lambda = 0, \mathbf{x} \neq \mathbf{0} \end{cases}$$

and  $H_0^{(1)}$  is the Hankel function of first kind and order zero. However, the explicit expression in (3.8) shows that  $G_\lambda(\mathbf{0})$  does not exist. So we formally propose a renormalized coupling constant  $\alpha = c^{-1} - G_0(\mathbf{0})$  and interpret  $G_0(\mathbf{0}) - G_\lambda(\mathbf{0})$  as

$$\begin{aligned} \lim_{\mathbf{x} \rightarrow \mathbf{0}} (G_0(\mathbf{0}) - G_\lambda(\mathbf{0})) &= \lim_{\mathbf{x} \rightarrow \mathbf{0}} \left( -\frac{\ln |\mathbf{x}|}{2\pi} - \frac{i}{4} H_0^{(1)}(\sqrt{\lambda}|\mathbf{x}|) \right) \\ &= \frac{1}{2\pi} \left( \ln \frac{\sqrt{\lambda}}{i} - \ln 2 + \gamma \right) \end{aligned}$$

where  $\gamma \approx 0.5772$  is the Euler–Mascheroni constant. So we obtain the resolvent formula of  $-\Delta_{\alpha, \{\mathbf{0}\}}$ , the one point scatterer at the origin, as follows.

$$(3.9) \quad (-\Delta_{\alpha, \{\mathbf{0}\}} - \lambda)^{-1}(\mathbf{x}, \mathbf{x}') = G_\lambda(\mathbf{x} - \mathbf{x}') + G_\lambda(\mathbf{x}) \left( \alpha + \frac{1}{2\pi} \left( \ln \frac{\sqrt{\lambda}}{i} - \ln 2 + \gamma \right) \right)^{-1} G_\lambda(\mathbf{x}') \\ \lambda \notin \sigma(-\Delta_{\alpha, \{\mathbf{0}\}}), \text{ Im } \sqrt{\lambda} > 0, \alpha \in \mathbb{R}$$

See Theorem 5.2 in [2] for a rigorous description of (3.9).

*Remark.* We do not need such a process in  $\mathbb{R}^1$  since the free resolvent  $G_\lambda(x) = e^{i\sqrt{\lambda}|x|}$  has a finite value at  $x = 0$ , so the model of 1-dimensional  $\delta$ -potentials [11] works without the renormalization.

**3.3.2. Finitely many point scatterers.** We formulate a Schrödinger operator with finitely many point scatterers using the theory of self-adjoint extensions. Then we consider infinitely many point scatterers as the limit of them under some conditions.

We will summarize some well-known results from self-adjoint extension theory [8] first. Suppose  $A$  is a densely defined, closed, symmetric operator in some Hilbert space  $\mathcal{H}$  with deficiency indices  $(N, N)$ ,  $N \in \mathbb{N}$ . If

$$A^* \phi_j(z) = z \phi_j(z), \quad \phi_j(z) \in D(A^*), \quad 1 \leq j \leq N, \quad z \in \mathbb{C} \setminus \mathbb{R},$$

we have the following result:

**Proposition 3.1.** *All self-adjoint extensions  $A_U$  of  $A$  may be parametrized by an  $N \times N$  complex-valued unitary matrix  $U$  where*

$$D(A_U) = \left\{ g + \sum_{j=1}^N c_j \left[ \phi_j(i) + \sum_{j'=1}^N U_{jj'} \phi_{j'}(-i) \right] \mid g \in D(A), \quad c_j \in \mathbb{C}, \quad j = 1, \dots, N \right\}$$

and

$$\begin{aligned} A_U \left( g + \sum_{j=1}^N c_j \left[ \phi_j(i) + \sum_{j'=1}^N U_{jj'} \phi_{j'}(-i) \right] \right) \\ = Ag + i \sum_{j=1}^N c_j \left[ \phi_j(i) - \sum_{j'=1}^N U_{jj'} \phi_{j'}(-i) \right]. \end{aligned}$$

Let  $B$  and  $C$  denote any self-adjoint extensions of  $A$ . Then we have  $\tilde{A}$ , the maximal common part of  $B$  and  $C$ , i.e.,  $\tilde{A} \subseteq B$ ,  $\tilde{A} \subseteq C$  and  $\tilde{A}$  extends any operator  $A'$  that satisfies  $A' \subseteq B$  and  $A' \subseteq C$ . Let  $M$ ,  $1 \leq M \leq N$  be the deficiency indices of  $\tilde{A}$  and let  $\{\phi_1(z), \dots, \phi_M(z)\}$  span the corresponding deficiency subspace of  $\tilde{A}$ , i.e.,

$$(3.10) \quad \tilde{A}^* \phi_j(z) = z \phi_j(z), \quad \phi_j(z) \in D(\tilde{A}^*), \quad 1 \leq j \leq M, \quad z \in \mathbb{C} \setminus \mathbb{R}$$

**Proposition 3.2** (Krein's formula). *Let  $A, B, C$ , and  $\tilde{A}$  be as above. Then*

$$(B - z)^{-1} - (C - z)^{-1} = \sum_{j,j'=1}^M \kappa_{jj'}(z) (\phi_j(\bar{z}), \bullet) \phi_{j'}(z), \quad z \in \rho(B) \cap \rho(C),$$

where the  $M \times M$  matrix  $\kappa(z)$  is nonsingular for  $z \in \rho(B) \cap \rho(C)$  and  $\kappa_{jj'}(z)$  and  $\phi_j(z)$  may be chosen to be analytic in  $z \in \rho(B) \cap \rho(C)$ . In addition,  $\phi_j(z)$  and  $\kappa_{jj'}(z)$  satisfy

$$\phi_j(z) = \phi_j(z_0) + (z - z_0)(C - z_0)^{-1} \phi_j(z_0), \quad j = 1, \dots, M, \quad z \in \rho(C)$$

and

$$(3.11) \quad [\kappa(z)^{-1}]_{jj'} = [\kappa(z')^{-1}]_{jj'} - (z - z')(\phi_j(\bar{z}), \phi_{j'}(z)), \\ j, j' = 1, \dots, M, \quad z, z' \in \rho(B) \cap \rho(C)$$

where  $\phi_j(z)$ ,  $1 \leq j \leq M$  are defined by (3.10).

We now formulate the finitely many point scatterers in  $\mathbb{R}^2$ . Let  $Y = \{\mathbf{y}_1, \dots, \mathbf{y}_N\} \subset \mathbb{R}^2$ . We consider the nonnegative operator

$$-\Delta|_{C_0^\infty(\mathbb{R}^2 \setminus Y)}$$

with  $P_Y$  its closure in  $L^2(\mathbb{R}^2)$ . Then we have

$$P_Y = -\Delta, \quad D(P_Y) = H_0^2(\mathbb{R}^2 \setminus Y)$$

and

$$P_Y^* = -\Delta, \quad D(P_Y^*) = \{g \in H_{\text{loc}}^2(\mathbb{R}^2 \setminus Y) \cap L^2(\mathbb{R}^2) \mid \Delta g \in L^2(\mathbb{R}^2)\}.$$

Then

$$P_Y^* \psi(\lambda) = \lambda \psi(\lambda), \quad \psi(\lambda) \in D(P_Y^*), \quad \lambda \in \mathbb{C} \setminus \mathbb{R}$$

has the solutions

$$\psi(\lambda) = G_\lambda(\bullet - \mathbf{y}_j), \quad j = 1, \dots, N$$

Therefore, we obtain

$$\ker(P_Y^* \mp i) = \{G_{\pm i, \mathbf{y}_j} \mid j = 1, \dots, N\}$$

where  $G_{\lambda, \mathbf{y}_j}$  is defined by

$$(3.12) \quad G_{\lambda, \mathbf{y}_j}(\mathbf{x}) = G_\lambda(\mathbf{x} - \mathbf{y}_j), \quad \mathbf{x} \neq \mathbf{y}_j, \quad j = 1, \dots, N.$$

Hence,  $P_Y$  has the deficiency indices  $(N, N)$ . By Proposition 3.1, this implies that all self-adjoint extensions of  $P_Y$  can be parametrized by  $N \times N$  unitary matrices  $U$ . More precisely, self-adjoint extensions  $P_{U,Y}$  of  $P_Y$  are given by

$$\begin{aligned} & D(P_{U,Y}) \\ &= \left\{ g + \sum_{j=1}^N c_j \left[ G_{i, \mathbf{y}_j} + \sum_{j'=1}^N U_{jj'} G_{-i, \mathbf{y}_{j'}} \right] \mid g \in D(P_Y), \quad c_j \in \mathbb{C}, \quad j = 1, \dots, N \right\} \end{aligned}$$

and

$$\begin{aligned} & P_{U,Y} \left( g + \sum_{j=1}^N c_j \left[ G_{i, \mathbf{y}_j} + \sum_{j'=1}^N U_{jj'} G_{-i, \mathbf{y}_{j'}} \right] \right) \\ &= Ag + i \sum_{j=1}^N c_j \left[ \phi_j(i) - \sum_{j'=1}^N U_{jj'} \phi_j(-i) \right] \end{aligned}$$

Note that  $U = -I$  corresponds to the free Hamiltonian  $H_{-I,Y} = -\Delta$  with  $D(H_{-I,Y}) = H^2(\mathbb{R}^2)$  since  $G_i - G_{-i} \in H^2(\mathbb{R}^2)$ .

Applying Krein's formula, we obtain

$$(3.13) \quad (P_{U,Y} - \lambda)^{-1} = (-\Delta - \lambda)^{-1} + \sum_{j,j'=1}^N [\kappa(\lambda)]_{jj'} (G_{\bar{\lambda}, \mathbf{y}_j}, \bullet) G_{\lambda, \mathbf{y}_{j'}} \\ \lambda \notin \sigma(P_{U,Y}), \quad U \neq -I$$

where

$$(3.14) \quad [\kappa(\lambda)^{-1}]_{jj'} - [\kappa(\lambda')^{-1}]_{jj'} = -(\lambda - \lambda') (G_{\bar{\lambda}, \mathbf{y}_j}, G_{\lambda', \mathbf{y}_{j'}}) \\ = G_{\lambda', \mathbf{y}_{j'}} - G_{\lambda, \mathbf{y}_j}$$

A straightforward computation then gives the relationship between two parameters  $U$  in Proposition 3.1 and  $\kappa(\lambda)$  in Proposition 3.2, namely,

$$U = -[\kappa(i)^{-1}\kappa(-i)]^T.$$

(See Chapter II.4 in [2].) Since Krein's formula (3.13) implies

$$\kappa(\lambda)^* = \kappa(\bar{\lambda}), \quad \lambda \notin \sigma(P_{U,Y}),$$

we conclude that unitarity of  $U$  is equivalent to the normality of  $\kappa(i)$ . Note that once  $\kappa(i)$  is determined,  $\kappa(\lambda)$  is given by (3.14).

Inspired by (3.9) we choose  $N$  parameters that only affect the diagonal entries of  $\kappa(\lambda)$ .

$$(3.15) \quad \begin{aligned} [\kappa(\lambda)^{-1}]_{jj'} &= [\Gamma_{\alpha,Y}(\lambda)]_{jj'} \\ &= \begin{cases} \alpha_j + \frac{1}{2\pi} \left( \ln \frac{\sqrt{\lambda}}{i} - \ln 2 + \gamma \right), & \text{if } j = j' \\ -G_\lambda(\mathbf{y}_{j'} - \mathbf{y}_j), & \text{if } j \neq j' \end{cases} \end{aligned}$$

which of course satisfies (3.14).

Then we have  $-\Delta_{\alpha,Y}$  with  $\alpha = (\alpha_1, \dots, \alpha_N) \in (-\infty, \infty]^N$  and the resolvent formula given by

$$(3.16) \quad (-\Delta_{\alpha,Y} - \lambda)^{-1} = G_\lambda + \sum_{j,j'=1}^N [\Gamma_{\alpha,Y}(\lambda)^{-1}]_{jj'} (G_{\lambda,\mathbf{y}'}, \bullet) G_{\lambda,\mathbf{y}}$$

where  $\Gamma_{\alpha,Y}(\lambda)$  is defined by (3.15).

**3.3.3. Point scatterers on a periodic structure.** Now we consider the point scatterers on a periodic structure. We will use the notation  $\mathbf{y}_1 = \mathbf{0}$ ,  $\mathbf{y}_2 = \mathbf{x}_0$ ,  $Y = \{\mathbf{y}_1, \mathbf{y}_2\}$ , and  $H = \Lambda + Y$  for simplicity. The whole process in this section can be also applied to the case of any  $N$  periodic point scatterers on  $\mathbb{R}^2$ .

We now investigate two kinds of operators:  $-\Delta_{\beta,H}$  with infinitely many point scatterers on  $H$ , and the decomposed “fiber”  $-\Delta_{\alpha,Y}(\mathbf{k})$ ,  $\mathbf{k} \in \mathcal{B}$  where

$$(3.17) \quad \alpha_j = \beta_{\mathbf{y}_j + \mathbf{v}_m} \in (-\infty, \infty], \quad j = 1, 2, \quad \mathbf{v}_m \in \Lambda.$$

First, we may consider  $-\Delta_{\alpha,H}$  as the limit of finitely many point scatterers, namely

$$(3.18) \quad (-\Delta_{\beta,H} - \lambda)^{-1} = G_\lambda + \sum_{j,j'=1}^{\infty} [\Gamma_{\beta,H}(\lambda)^{-1}]_{jj'} (G_{\lambda,\mathbf{y}_{j'}}, \bullet) G_{\lambda,\mathbf{y}_j}$$

where  $\Gamma_{\beta,H}(\lambda)$  is a closed operator in  $l^2(H)$  given by

$$[\Gamma_{\beta,H}(\lambda)]_{jj'} = \begin{cases} \beta_j + \frac{1}{2\pi} \left( \ln \frac{\sqrt{\lambda}}{i} - \ln 2 + \gamma \right), & \text{if } j = j', \quad j, j' \in \mathbb{N} \\ -G_\lambda(\mathbf{y}_{j'} - \mathbf{y}_j), & \text{if } j \neq j', \quad j, j' \in \mathbb{N} \end{cases}$$

See Theorem 4.1 in [2] for the complete proof.

On the other hand, for the decomposed operator  $-\Delta_{\alpha,Y}(\mathbf{k})$ , we will exploit the idea of renormalization introduced in 3.3.1 more rigorously with the case of infinitely many point scatterers on a periodic structure since they are obtained by eventually the same process.



In order to formulate point scatterers on a honeycomb lattice  $H$ , we first consider a periodic potential  $V$  formally defined by

$$V(\mathbf{x}) = \sum_{j=1}^2 \sum_{\mathbf{v} \in \Lambda} c_j \delta(\mathbf{x} - \mathbf{v} - \mathbf{y}_j), \quad c_j \in \mathbb{R},$$

which provides a simplified model of a crystal composed by two kinds of atoms whose nuclei are located on  $H$ .

Then

$$(3.19) \quad V_{\mathbf{m}} = -\frac{1}{|\Gamma|} \sum_{j=1}^2 c_j e^{-i\xi_{\mathbf{m}} \cdot \mathbf{y}_j}, \quad \mathbf{m} \in \mathbb{Z}^2$$

Hence, we obtain the central equation for  $V(\mathbf{x})$  from (3.6). For  $g \in l_0^2(\Lambda^*) = \{h \in l^2(\Lambda^*) \mid \text{supp } h \text{ is finite}\}$ ,

$$(3.20) \quad \hat{P}(\mathbf{k})g(\xi_{\mathbf{m}}) = |\xi_{\mathbf{m}} + \mathbf{k}|^2 g(\xi_{\mathbf{m}}) - \frac{1}{|\Gamma|} \sum_{j=1}^2 \left[ c_j e^{-i\xi_{\mathbf{m}} \cdot \mathbf{y}_j} \sum_{\mathbf{m}' \in \mathbb{Z}^2} e^{i\xi_{\mathbf{m}'} \cdot \mathbf{y}_j} g(\xi_{\mathbf{m}'} \right]$$

However, this is obviously not a well-defined self-adjoint operator in  $l^2(\Lambda^*)$ . So we propose a renormalization by the momentum cutoff  $|\xi_{\mathbf{m}} + \mathbf{k}| < \omega$ . Then we consider the coupling constants  $c_j$  as a function of  $\omega$  so that they approach zero as  $\omega \rightarrow \infty$ . In other words, this renormalization process will make the summation in (3.20) converge in some sense so we can define the point scatterer as a well-defined self-adjoint operator.

Before stating the resolvent formula of point scatterers, we need two lemmas each of which is related to so-called the Weinstein-Aronszajn determinant and the Poisson summation formula, respectively. See Lemma B.5 and Lemma III.4.4 in [2].

**Lemma 3.3.** *Let  $\mathcal{H}$  be a separable Hilbert space, let  $A$  be a closed operator in  $\mathcal{H}$  and  $\phi_j, \psi_j \in \mathcal{H}$ ,  $j = 1 \dots, N$ . Then*

$$\begin{aligned} & \left[ A + \sum_{j=1}^N (\phi_j, \bullet) \psi_j - z \right]^{-1} \\ &= (A - z)^{-1} - \sum_{j=1}^N [M(z)^{-1}]_{jj'} ([ (A - z)^{-1} ]^* \psi_j, \bullet) (A - z)^{-1} \psi_{j'} \end{aligned}$$

where

$$M(z) = [\delta_{jj'} + (\phi_{j'}, (A - z)^{-1} \psi_j)]_{j,j'=1}^N$$

**Lemma 3.4** (Poisson summation formula). *Let  $\lambda \in \mathbb{C}$ ,  $\text{Im } \sqrt{\lambda} > 0$ , and  $\mathbf{k} \in \mathcal{B}$ . Then*

$$\begin{aligned} (2\pi)^{-2} \lim_{\omega \rightarrow \infty} & \left[ \sum_{\substack{m \in \mathbb{Z}^2 \\ |\xi_{\mathbf{m}} + \mathbf{k}| \leq \omega}} \frac{|\mathcal{B}|}{|\xi_{\mathbf{m}} + \mathbf{k}|^2 - \lambda} - 2\pi \ln \omega \right] \\ &= \sum_{\mathbf{m} \in \mathbb{Z}^2 \setminus \{\mathbf{0}\}} G_{\lambda}(\mathbf{x}_{\mathbf{m}}) e^{-i\mathbf{k} \cdot \mathbf{x}_{\mathbf{m}}} + \frac{1}{2\pi} \ln \frac{\sqrt{\lambda}}{i} \end{aligned}$$

We now obtain the resolvent of point scatterers as an application of Lemma 3.3. See Theorem III.1.4.1 and Theorem III.4.3 in [2] for the proof. The coupling constant  $\alpha_j$  in this proposition corresponds to  $\alpha_j + \frac{\gamma}{2\pi}$  in [2].

**Proposition 3.5.** *Let  $\hat{P}^\omega(\mathbf{k})$  be a self-adjoint operator such that*

$$(\hat{P}^\omega(\mathbf{k})g)(\xi_{\mathbf{m}}) = |\xi_{\mathbf{m}} + \mathbf{k}|^2 g(\xi_{\mathbf{m}}) - \frac{1}{|\Gamma|} \sum_{j=1}^2 \left[ c_j(\omega) (\phi_{\mathbf{y}_j}^\omega(\mathbf{k}), g) \phi_{\mathbf{y}_j}^\omega(\mathbf{k}) \right]$$

where  $(\bullet, \bullet)$  is the inner product in  $l^2(\Lambda^*)$  and  $\phi_{\mathbf{y}_j}^\omega(\mathbf{k})$  is the function

$$\phi_{\mathbf{y}_j}^\omega(\mathbf{k}, \xi_{\mathbf{m}}) = \chi_\omega(\xi_{\mathbf{m}} + \mathbf{k}) e^{-i(\xi_{\mathbf{m}} + \mathbf{k}) \cdot \mathbf{y}_j}$$

with a domain

$$D(\hat{P}^\omega(\mathbf{k})) = D(-\hat{\Delta}(\mathbf{k})) = \left\{ g \in l^2(\Lambda^*) \left| \sum_{\mathbf{m} \in \mathbb{Z}^2} |\xi_{\mathbf{m}} + \mathbf{k}|^4 g(\xi_{\mathbf{m}})^2 < \infty \right. \right\}.$$

If

$$c_j(\omega) = \left( \alpha_j + \frac{\ln \omega - \ln 2}{2\pi} \right)^{-1}, \quad \alpha_j \in (-\infty, \infty], \quad \omega > 0$$

then for all  $\mathbf{k} \in \mathcal{B}$ ,  $\hat{P}^\omega(\mathbf{k})$  converges in norm resolvent sense as  $\omega \rightarrow \infty$  to a self-adjoint operator  $-\hat{\Delta}_{\alpha, Y}(\mathbf{k})$  with resolvent

(3.21)

$$\begin{aligned} (-\hat{\Delta}_{\alpha, Y}(\mathbf{k}) - \lambda)^{-1} &= G_\lambda(\mathbf{k}) + \frac{1}{|\Gamma|} \sum_{j=1}^2 [\Gamma_{\alpha, Y}(\lambda, \mathbf{k})^{-1}]_{jj'} (F_{\lambda, \mathbf{y}_j}(\mathbf{k}), \bullet) F_{\lambda, \mathbf{y}_{j'}}(\mathbf{k}), \\ &\quad \lambda \notin \{ |\xi_{\mathbf{m}} + \mathbf{k}|^2 \mid \xi_{\mathbf{m}} \in \Lambda^* \}, \quad \alpha = (\alpha_1, \alpha_2) \end{aligned}$$

where

$$(3.22) \quad g_\lambda(\mathbf{x}, \mathbf{k}) = \begin{cases} \frac{1}{|\Gamma|} \sum_{\mathbf{m} \in \mathbb{Z}^2} \frac{e^{i(\xi_{\mathbf{m}} + \mathbf{k}) \cdot \mathbf{x}}}{|\xi_{\mathbf{m}}^2 + \mathbf{k}|^2 - \lambda} & \text{if } \mathbf{x} \notin \Lambda \\ \frac{1}{|\Gamma|} \lim_{\omega \rightarrow \infty} \left[ \sum_{\substack{\mathbf{m} \in \mathbb{Z}^2 \\ |\xi_{\mathbf{m}} + \mathbf{k}| \leq \omega}} \frac{1}{|\xi_{\mathbf{m}} + \mathbf{k}|^2 - \lambda} - \frac{2\pi}{|\mathcal{B}|} \ln \omega \right] & \text{if } \mathbf{x} \in \Lambda \end{cases}$$

$$(3.23) \quad \Gamma_{\alpha, Y}(\lambda, \mathbf{k}) = [\alpha_j \delta_{jj'} - g_\lambda(\mathbf{y}_{j'} - \mathbf{y}_j, \mathbf{k})]_{j, j'=1}^N$$

and

$$(3.24) \quad F_{\lambda, \mathbf{y}_j}(\mathbf{k}, \xi_{\mathbf{m}}) = \frac{e^{-i(\xi_{\mathbf{m}} + \mathbf{k}) \cdot \mathbf{y}_j}}{|\xi_{\mathbf{m}} + \mathbf{k}|^2 - \lambda}$$

and  $G_\lambda(\mathbf{k}) : l^2(\Lambda^*) \rightarrow l^2(\Lambda^*)$  is the multiplication operator

$$(G_\lambda(\mathbf{k})g)(\xi_{\mathbf{m}}) = (|\xi_{\mathbf{m}} + \mathbf{k}|^2 - \lambda)^{-1} g(\xi_{\mathbf{m}})$$

*Proof.* By Lemma 3.3, for  $\lambda \notin \sigma(\hat{P}^\omega(\mathbf{k}))$ , we have the integral kernel

$$(\hat{P}^\omega(\mathbf{k}) - \lambda)^{-1}(\mathbf{x}, \mathbf{x}') = G_\lambda(\mathbf{k})(\mathbf{x} - \mathbf{x}') + \sum_{j,j'=1}^2 [\Gamma_{\Lambda,Y}^\omega(\lambda, \mathbf{k})^{-1}]_{jj'} (G_\lambda(\mathbf{k}) \overline{\phi_{\mathbf{y}_j}^\omega(\mathbf{k})})(\mathbf{x}) (G_\lambda(\mathbf{k}) \phi_{\mathbf{y}_{j'}}^\omega(\mathbf{k}))(\mathbf{x}')$$

where  $\lambda \notin \{|\xi_{\mathbf{m}} + \mathbf{k}|^2 \mid \xi_{\mathbf{m}} \in \Lambda^*\}$  and

$$\Gamma_{\Lambda,Y}^\omega(\lambda, \mathbf{k}) = \left[ |\Gamma| c_j(\omega)^{-1} \delta_{jj'} - \left( \phi_{\mathbf{y}_{j'}}^\omega(\mathbf{k}), G_\lambda(\mathbf{k}) \phi_{\mathbf{y}_j}^\omega(\mathbf{k}) \right) \right]_{j,j'=1}^2.$$

By Lemma 3.4, we observe that the  $j$ -th diagonal entry of  $\Gamma_{\Lambda,Y}^\omega(\lambda, \mathbf{k})$  is equal to

$$\begin{aligned} [\Gamma_{\Lambda,Y}^\omega(\lambda, \mathbf{k})]_{jj} &= |\Gamma| c_j(\omega)^{-1} - \left( \phi_{\mathbf{y}_j}^\omega(\mathbf{k}), G_\lambda(\mathbf{k}) \phi_{\mathbf{y}_j}^\omega(\mathbf{k}) \right) \\ &= |\Gamma| \left[ \alpha_j + \frac{\ln \omega - \ln 2}{2\pi} - (2\pi)^{-2} \sum_{\substack{m \in \mathbb{Z}^2 \\ |\xi_{\mathbf{m}} + \mathbf{k}| \leq \omega}} \frac{|\mathcal{B}|}{|\xi_{\mathbf{m}} + \mathbf{k}|^2 - \lambda} \right] \\ &\xrightarrow{\omega \rightarrow \infty} |\Gamma| [\alpha_j - g_\lambda(\mathbf{0}, \mathbf{k})] \end{aligned}$$

In addition, the off-diagonal elements  $[\Gamma_{\Lambda,Y}^\omega(\lambda, \mathbf{k})]_{jj'}$ ,  $j \neq j'$  are equal to

$$\begin{aligned} [\Gamma_{\Lambda,Y}^\omega(\lambda, \mathbf{k})]_{jj'} &= - \left( \phi_{\mathbf{y}_{j'}}^\omega(\mathbf{k}), G_\lambda(\mathbf{k}) \phi_{\mathbf{y}_j}^\omega(\mathbf{k}) \right) \\ &= - \sum_{\substack{m \in \mathbb{Z}^2 \\ |\xi_{\mathbf{m}} + \mathbf{k}| \leq \omega}} \frac{e^{i(\xi_{\mathbf{m}} + \mathbf{k}) \cdot (\mathbf{y}_{j'} - \mathbf{y}_j)}}{|\xi_{\mathbf{m}} + \mathbf{k}|^2 - \lambda} \\ &\xrightarrow{\omega \rightarrow \infty} -|\Gamma| g_\lambda(\mathbf{y}_{j'} - \mathbf{y}_j, \mathbf{k}), \quad j \neq j', \end{aligned}$$

On the other hand, we observe

$$\left\| \left( \overline{G_\lambda(\mathbf{k}) \phi_{\mathbf{y}_j}^\omega(\mathbf{k})}, \bullet \right) G_\lambda(\mathbf{k}) \phi_{\mathbf{y}_{j'}}^\omega(\mathbf{k}) - \left( \overline{F_{\lambda, \mathbf{y}_j}(\mathbf{k})}, \bullet \right) F_{\lambda, \mathbf{y}_{j'}}(\mathbf{k}) \right\|_{l^2 \rightarrow l^2} \xrightarrow{\omega \rightarrow \infty} 0$$

Hence, we obtain the following convergence in norm resolvent sense.

$$(\hat{P}^\omega(\mathbf{k}) - \lambda)^{-1} \xrightarrow{\omega \rightarrow \infty} G_\lambda(\mathbf{k}) + \frac{1}{|\Gamma|} \sum_{j=1}^2 [\Gamma_{\Lambda,Y}^\omega(\lambda, \mathbf{k})^{-1}]_{jj'} (F_{\lambda, \mathbf{y}_j}(\mathbf{k}), \bullet) F_{\lambda, \mathbf{y}_{j'}}(\mathbf{k})$$

Furthermore,  $-\hat{\Delta}_{\alpha,Y}(\mathbf{k})$  is self-adjoint since the resolvent formula (3.21) implies

$$\begin{aligned} (-\hat{\Delta}_{\alpha,Y}(\mathbf{k})^* - \bar{\lambda})^{-1} &= [(-\hat{\Delta}_{\alpha,Y}(\mathbf{k}) - \lambda)^*]^{-1} \\ &= [(-\hat{\Delta}_{\alpha,Y}(\mathbf{k}) - \lambda)^{-1}]^* \\ &= (-\hat{\Delta}_{\alpha,Y}(\mathbf{k}) - \bar{\lambda})^{-1}, \quad \lambda \notin \sigma(-\hat{\Delta}_{\alpha,Y}(\mathbf{k})) \end{aligned}$$

□

Moreover, we have the corresponding formula of the decomposed operator in  $L_{\mathbf{k}}^2(\Gamma)$ , which will be used frequently in the next section. See Theorem III.1.4.3 and Theorem III.4.3 in [2].

**Proposition 3.6.** *Let  $\alpha = (\alpha_1, \alpha_2) \in (-\infty, \infty]^2$ . For  $\lambda \notin \sigma(-\Delta(\mathbf{k}))$ , the resolvent  $(-\Delta_{\alpha,Y}(\mathbf{k}) - \lambda)^{-1} : L_{\mathbf{k}}^2(\Gamma) \rightarrow L_{\mathbf{k}}^2(\Gamma)$  is defined by*

$$(3.25) \quad (-\Delta_{\alpha,Y}(\mathbf{k}) - \lambda)^{-1} f(\mathbf{x}) = (-\Delta(\mathbf{k}) - \lambda)^{-1} f(\mathbf{x}) + \frac{1}{|\mathcal{B}|} \sum_{j,j'=1}^2 [\Gamma_{\alpha,Y}(\lambda, \mathbf{k})^{-1}]_{jj'} \left( g_{\lambda}(\bullet - \mathbf{y}_j, \mathbf{k}), f \right) g_{\lambda}(\mathbf{x} - \mathbf{y}_{j'}, \mathbf{k})$$

where  $g_{\lambda}(x, \mathbf{k})$  and  $\Gamma_{\alpha,Y}(\lambda, \mathbf{k})$  are defined in (3.22) and (3.23), respectively.

If the infinite sequence of coupling constants  $\beta$  is defined by (3.17), we observe the relationship between the Fourier transform of the full Hamiltonian  $-\Delta_{\beta,H}$  in (3.18) and the decomposed operator  $-\hat{\Delta}_{\alpha,Y}(\mathbf{k})$  in (3.21). Note that this result corresponds to the Floquet theory for smooth potentials in Section 3.2. See Theorem III.1.4.3 and Theorem III.4.5 in [2].

**Proposition 3.7.** *Let  $\alpha = (\alpha, \alpha)$  and  $\beta = (\alpha, \alpha, \dots)$  where  $\alpha \in (-\infty, \infty]$ . Then  $-\hat{\Delta}_{\beta,H}$  is unitarily equivalent to  $\int_{\mathcal{B}}^{\otimes} -\hat{\Delta}_{\alpha,Y}(\mathbf{k}) d\mathbf{k}$  so*

$$(3.26) \quad \bigcup_{\mathbf{k} \in \mathcal{B}} \sigma(-\Delta_{\alpha,Y}(\mathbf{k})) = \bigcup_{\mathbf{k} \in \mathcal{B}} \sigma(-\hat{\Delta}_{\alpha,Y}(\mathbf{k})) = \sigma(-\hat{\Delta}_{\beta,H}) = \sigma(-\Delta_{\beta,H})$$

where the decomposed self-adjoint operator  $-\Delta_{\alpha,Y}(\mathbf{k})$  has a purely discrete spectrum. Hence, as in the periodic potential case the eigenvalues of  $\Delta_{\beta,H}$  also form a band structure if the dependence in  $\mathbf{k}$  is continuous.

On the other hand, Proposition 3.6 provides an additional information on the domain of  $-\Delta_{\alpha,Y}(\mathbf{k})$ .

**Proposition 3.8.** *Let  $\psi \in D(-\Delta_{\alpha,Y}(\mathbf{k}))$ . Then for any  $\lambda \notin \sigma(-\Delta(\mathbf{k})) \cup \sigma(-\Delta_{\alpha,Y}(\mathbf{k}))$ , there exists a unique  $\phi_{\lambda} \in H_{\mathbf{k}}^2(\mathbb{R}^2)$  such that*

$$(3.27) \quad \psi(\mathbf{x}) = \phi_{\lambda}(\mathbf{x}) + \frac{1}{|\mathcal{B}|} \sum_{j,j'=1}^2 [\Gamma_{\alpha,Y}(\lambda, \mathbf{k})^{-1}]_{jj'} \phi_{\lambda}(\mathbf{y}_j) g_{\lambda}(\mathbf{x} - \mathbf{y}_{j'}, \mathbf{k}).$$

In addition,

$$(-\Delta_{\alpha,Y}(\mathbf{k}) - \lambda)^{-1} \psi = (-\Delta(\mathbf{k}) - \lambda)^{-1} \phi_{\lambda}.$$

*Proof.* Since  $\lambda \notin \sigma(-\Delta(\mathbf{k})) \cup \sigma(-\Delta_{\alpha,Y}(\mathbf{k}))$ , we can define  $\phi_{\lambda} \in H_{\mathbf{k}}^2(\mathbb{R}^2)$  by

$$\phi_{\lambda} = (-\Delta(\mathbf{k}) - \lambda)^{-1} (-\Delta_{\alpha,Y}(\mathbf{k}) - \lambda) \psi.$$

Since  $\psi = (-\Delta_{\alpha,Y}(\mathbf{k}) - \lambda)^{-1} (-\Delta(\mathbf{k}) - \lambda) \phi_{\lambda}$ , we obtain (3.27) with the resolvent formula given in Proposition 3.6. Note that we can define  $\phi_{\lambda}(\mathbf{x})$  pointwise at each  $\mathbf{x} \in \Gamma$  since  $H_{\mathbf{k}}^2(\mathbb{R}^2) \subset C^0(\mathbb{R}^2)$  by Sobolev Embedding theorem.

To prove uniqueness, suppose  $\psi \equiv 0$ . Note that  $g_{\lambda}(\bullet, \mathbf{k}) \notin H^2$ . Since  $\Gamma_{\alpha,Y}(\lambda, \mathbf{k})^{-1}$  is an invertible matrix, we observe that

$$\sum_{j=1}^2 [\Gamma_{\alpha,Y}(\lambda, \mathbf{k})^{-1}]_{jj'} \phi_{\lambda}(\mathbf{y}_j) = 0, \quad 1 \leq j' \leq 2$$

if and only if  $\phi_{\lambda}(\mathbf{y}_j) = 0$ ,  $1 \leq j \leq 2$ . So we conclude that  $\psi \equiv 0$  implies  $\phi_{\lambda} \equiv 0$ , which proves the uniqueness.  $\square$

## 4. HONEYCOMB LATTICE POINT SCATTERERS

Now we compare the decomposed point scatterer  $-\Delta_{\alpha,Y}(\mathbf{k})$  to a decomposed linear Schrödinger operator  $-\Delta(\mathbf{k}) + V$  when the set of scattering points  $H = Y + \Lambda$  and the potential  $V$  share some properties induced by the honeycomb lattice defined in [1].

**Definition 4.1** (Honeycomb lattice potentials).  $V \in C^\infty(\mathbb{R}^2; \mathbb{R})$  is a honeycomb lattice potential if there exists  $\mathbf{y} \in \Gamma$  such that

- (1)  $V$  is  $\mathcal{T}_{\mathbf{v}}$ -invariant for all  $\mathbf{v} \in \Lambda$  where  $\mathcal{T}_{\mathbf{v}}V(\mathbf{x}) = V(\mathbf{x} + \mathbf{v})$  is the translation along  $\mathbf{v}$ , i.e.  $V(\mathbf{x} + \mathbf{v}) = V(\mathbf{x})$
- (2)  $V$  is  $\mathcal{I}_{\mathbf{y}}$ -invariant, where  $\mathcal{I}_{\mathbf{y}}V(\mathbf{x}) = V(2\mathbf{y} - \mathbf{x})$  is the inversion with respect to  $\mathbf{y}$ , i.e.  $V(2\mathbf{y} - \mathbf{x}) = V(\mathbf{x})$
- (3)  $\tilde{V}$  is  $\mathcal{R}_{\mathbf{y}}$ -invariant where  $\mathcal{R}_{\mathbf{y}}V(\mathbf{x}) = V(R(\mathbf{x} - \mathbf{y}) + \mathbf{y})$  is the  $\frac{2\pi}{3}$ -rotation with respect to  $\mathbf{y}$  with

$$(4.1) \quad R = \frac{1}{2} \begin{bmatrix} -1 & -\sqrt{3} \\ \sqrt{3} & -1 \end{bmatrix}$$

$$\text{i.e. } V(R(\mathbf{x} - \mathbf{y}) + \mathbf{y}) = V(\mathbf{x})$$

*Remark.* Since the Laplacian is invariant under  $\mathcal{T}_{\mathbf{v}}, \mathcal{I}_{\mathbf{y}}$  and  $\mathcal{R}_{\mathbf{y}}$ , these operations only affect the Floquet boundary condition whenever  $V$  is a honeycomb lattice potential. Therefore,

$$\begin{aligned} \mathcal{T}_{\mathbf{v}}(-\Delta(\mathbf{k}) + V)f &= (-\Delta(\mathbf{k}) + V)\mathcal{T}_{\mathbf{v}}f, \quad \mathbf{v} \in \Lambda \\ \mathcal{I}_{\mathbf{y}}(-\Delta(\mathbf{k}) + V)f &= (-\Delta(-\mathbf{k}) + V)\mathcal{I}_{\mathbf{y}}f \\ \mathcal{R}_{\mathbf{y}}(-\Delta(\mathbf{k}) + V)f &= (-\Delta(R^*\mathbf{k}) + V)\mathcal{R}_{\mathbf{y}}f \end{aligned}$$

Similarly, we can redefine a honeycomb lattice  $H = Y + \Lambda$  and the corresponding point scatterer  $-\Delta_{\alpha,Y}(\mathbf{k})$  in a generalized manner. Then it also satisfies the properties of  $-\Delta + V$  induced by the periodicity and symmetry of honeycomb lattices.

**Definition 4.2** (Generalized Honeycomb Lattices).  $X \subset \mathbb{R}^2$  is a generalized honeycomb lattice if there exists  $\mathbf{y} \in \Gamma$  such that

- (1)  $X$  is  $\Lambda$ -periodic, i.e.  $X + \mathbf{v} = X$ ,  $\mathbf{v} \in \Lambda$
- (2)  $X$  is inversion-symmetric with respect to  $\mathbf{y}$ , i.e.  $2\mathbf{y} - X = X$
- (3)  $X$  is  $\frac{2\pi}{3}$ -rotation invariant with respect to  $\mathbf{y}$ . i.e.  $R(X - \mathbf{y}) + \mathbf{y} = X$  where  $R$  is given by (4.1).

*Remark.* The honeycomb lattice  $H$  defined in Section 2 is also a generalized honeycomb lattice with  $\mathbf{y} = \frac{1}{3}(\mathbf{v}_1 + \mathbf{v}_2)$ .

**Definition 4.3** (Honeycomb Lattice Point Scatterers).  $-\Delta_{\alpha,Y}(\mathbf{k})$  is a honeycomb lattice point scatterer if the following conditions hold:

- (1)  $Y + \Lambda$  is a generalized honeycomb lattice with some  $\mathbf{y} \in \Gamma$  as the origin for the inversion and  $\frac{2\pi}{3}$ -rotation invariance.
- (2) The coupling constant at each point is invariant under the inversion with respect to  $\mathbf{y}$ , i.e.  $2\mathbf{y} - \mathbf{y}_j - \mathbf{y}_{j'} \in \Lambda$  implies  $\alpha_j = \alpha_{j'}$ .
- (3) The coupling constant at each point is invariant under the  $\frac{2\pi}{3}$ -rotation with respect to  $\mathbf{y}$ , i.e.  $R(\mathbf{y}_j - \mathbf{y}) + \mathbf{y} - \mathbf{y}_{j'} \in \Lambda$  implies  $\alpha_j = \alpha_{j'}$ .

**Proposition 4.1.** *Suppose  $-\Delta_{\alpha,Y}(\mathbf{k})$  is a honeycomb lattice point scatterer with some  $\mathbf{y} \in \Gamma$  as the origin for the inversion and  $\frac{2\pi}{3}$ -rotation invariance. For  $\psi \in D(-\Delta_{\alpha,Y}(\mathbf{k}))$ ,*

$$\begin{aligned}\mathcal{T}_{\mathbf{v}}\Delta_{\alpha,Y}(\mathbf{k})\psi &= \Delta_{\alpha,Y}(\mathbf{k})\mathcal{T}_{\mathbf{v}}\psi, \quad \mathbf{v} \in \Lambda \\ \mathcal{I}_{\mathbf{y}}\Delta_{\alpha,Y}(\mathbf{k})\psi &= \Delta_{\alpha,Y}(-\mathbf{k})\mathcal{I}_{\mathbf{y}}\psi \\ \mathcal{R}_{\mathbf{y}}\Delta_{\alpha,Y}(\mathbf{k})\psi &= \Delta_{\alpha,Y}(R^*\mathbf{k})\mathcal{R}_{\mathbf{y}}\psi\end{aligned}$$

*Proof.* Let  $\psi \in D(-\Delta_{\alpha,Y}(\mathbf{k}))$  and choose any  $\lambda \notin \sigma(-\Delta(\mathbf{k})) \cup \sigma(-\Delta_{\alpha,Y}(\mathbf{k}))$ . We can define  $\phi_\lambda \in H_{\mathbf{k}}^2(\mathbb{R}^2)$  as in (3.27). Since  $g_\lambda(\bullet, \mathbf{k}) \in L_{\mathbf{k}}^2$ , for  $\mathbf{v} \in \Lambda$ ,

$$\begin{aligned}\mathcal{T}_{\mathbf{v}}(-\Delta_{\alpha,Y}(\mathbf{k}) - \lambda)\psi &= \mathcal{T}_{\mathbf{v}}(-\Delta(\mathbf{k}) - \lambda)\phi_\lambda \\ &= (-\Delta(\mathbf{k}) - \lambda)\mathcal{T}_{\mathbf{v}}\phi_\lambda \\ &= (-\Delta_{\alpha,Y}(\mathbf{k}) - \lambda) \left[ \mathcal{T}_{\mathbf{v}}\phi_\lambda + \frac{1}{|\mathcal{B}|} \sum_{j,j'=1}^N [\Gamma_{\alpha,Y}(\lambda, \mathbf{k})^{-1}]_{jj'} (\mathcal{T}_{\mathbf{v}}\phi_\lambda)(\mathbf{y}_j) g_\lambda(\mathbf{x} - \mathbf{y}_{j'}, \mathbf{k}) \right] \\ &= (-\Delta_{\alpha,Y}(\mathbf{k}) - \lambda) \left[ \mathcal{T}_{\mathbf{v}}\phi_\lambda + \frac{1}{|\mathcal{B}|} \sum_{j,j'=1}^N [\Gamma_{\alpha,Y}(\lambda, \mathbf{k})^{-1}]_{jj'} \phi_\lambda(\mathbf{y}_j) (\mathcal{T}_{\mathbf{v}}g_\lambda)(\mathbf{x} - \mathbf{y}_{j'}, \mathbf{k}) \right] \\ &= (-\Delta_{\alpha,Y}(\mathbf{k}) - \lambda)\mathcal{T}_{\mathbf{v}}\psi\end{aligned}$$

In addition, we observe

$$\begin{aligned}\mathcal{I}_{\mathbf{y}}(-\Delta_{\alpha,Y}(\mathbf{k}) - \lambda)\psi &= \mathcal{I}_{\mathbf{y}}(-\Delta(\mathbf{k}) - \lambda)\phi_\lambda \\ &= (-\Delta(-\mathbf{k}) - \lambda)\mathcal{I}_{\mathbf{y}}\phi_\lambda \\ &= (-\Delta_{\alpha,Y}(-\mathbf{k}) - \lambda) \left[ \mathcal{I}_{\mathbf{y}}\phi_\lambda + \frac{1}{|\mathcal{B}|} \sum_{j,j'=1}^N [\Gamma_{\alpha,Y}(\lambda, \mathbf{k})^{-1}]_{jj'} (\mathcal{I}_{\mathbf{y}}\phi_\lambda)(\mathbf{y}_j) g_\lambda(\mathbf{x} - \mathbf{y}_{j'}, \mathbf{k}) \right] \\ &= (-\Delta_{\alpha,Y}(-\mathbf{k}) - \lambda) \left[ \mathcal{I}_{\mathbf{y}}\phi_\lambda + \frac{1}{|\mathcal{B}|} \sum_{l,l'=1}^N [\Gamma_{\alpha,Y}(\lambda, -\mathbf{k})^{-1}]_{ll'} \phi_\lambda(\mathbf{y}'_l) (\mathcal{I}_{\mathbf{y}'}g_\lambda)(\mathbf{x} - \mathbf{y}'_{l'}, -\mathbf{k}) \right] \\ &= (-\Delta_{\alpha,Y}(-\mathbf{k}) - \lambda)\mathcal{I}_{\mathbf{y}}\psi\end{aligned}$$

by rearranging  $Y = \{\mathbf{y}_1, \dots, \mathbf{y}_N\} = \{\mathbf{y}'_1, \dots, \mathbf{y}'_N\}$  so that

$$2\mathbf{y} - \mathbf{y}_j - \mathbf{y}'_l \in \Lambda, \quad 2\mathbf{y} - \mathbf{y}_{j'} - \mathbf{y}'_{l'} \in \Lambda$$

Similarly, we prove the rotation property as in the inversion case by rearranging  $Y = \{\mathbf{y}_1, \dots, \mathbf{y}_N\} = \{\mathbf{y}'_1, \dots, \mathbf{y}'_N\}$  so that

$$R(\mathbf{y}_j - \mathbf{y}) + \mathbf{y} - \mathbf{y}'_l \in \Lambda, \quad R(\mathbf{y}_{j'} - \mathbf{y}) + \mathbf{y} - \mathbf{y}'_{l'} \in \Lambda$$

Hence,

$$\mathcal{R}_{\mathbf{y}}(-\Delta_{\alpha,Y}(\mathbf{k}) - \lambda)\psi = (-\Delta_{\alpha,Y}(R^*\mathbf{k}) - \lambda)\mathcal{R}_{\mathbf{y}}\psi$$

This concludes the proof.  $\square$

**4.1. Point scatterers on the triangular lattice.** In this section, we first summarize several known results for the point scatterers on a periodic lattice with only one scatterer in the fundamental domain. See Chapter III.4 of [2] for more details. Then we observe the spectral properties of the triangular lattice point scatter as direct applications of those results.

Suppose there is one point scatterer on  $\Gamma$ , say at  $\mathbf{0}$ . Then we can classify all the eigenvalues of  $-\Delta_{\alpha, \{\mathbf{0}\}}(\mathbf{k})$  into two categories: the perturbed eigenvalues

$$\lambda \in \sigma(-\Delta_{\alpha, \{\mathbf{0}\}}(\mathbf{k})) \setminus \sigma(-\Delta(\mathbf{k}))$$

and the unperturbed eigenvalues

$$\lambda \in \sigma(-\Delta_{\alpha, \{\mathbf{0}\}}(\mathbf{k})) \cap \sigma(-\Delta(\mathbf{k})).$$

Applying Proposition 3.6, to the one periodic point scatterer model, we obtain the perturbed eigenvalues of triangular lattice point scatterer if and only if the  $1 \times 1$  matrix or scalar  $\Gamma_{\alpha, \{\mathbf{0}\}}(\lambda, \mathbf{k})$  in (3.23) is equal to zero. In other words,  $\lambda$  is a perturbed eigenvalue of  $-\Delta_{\alpha, \{\mathbf{0}\}}(\mathbf{k})$  if and only if

$$(4.2) \quad \alpha = g_\lambda(\mathbf{0}, \mathbf{k})$$

where  $g_\lambda$  is defined in (3.22), or equivalently,

$$(4.3) \quad |\Gamma|\alpha = \lim_{\omega \rightarrow \infty} \left[ \sum_{\substack{\mathbf{m} \in \mathbb{Z}^2 \\ |\xi_{\mathbf{m}} + \mathbf{k}| \leq \omega}} \frac{1}{|\xi_{\mathbf{m}} + \mathbf{k}|^2 - \lambda} - \frac{2\pi}{|\mathcal{B}|} \ln \omega \right].$$

In addition, every perturbed eigenvalue  $\lambda$  satisfies  $\text{mult}(\lambda, -\Delta_{\alpha, \{\mathbf{0}\}}(\mathbf{k})) = 1$  with the corresponding eigenfunction  $g_\lambda(\bullet, \mathbf{k})$ .

*Remark.* We may use a simpler summation formula (4.4) equivalent to the limit and partial sum notation (4.3):

$$(4.4) \quad |\Gamma|(\alpha + \alpha_0) = \sum_{\mathbf{m} \in \mathbb{Z}^2} \left[ \frac{1}{|\xi_{\mathbf{m}} + \mathbf{k}|^2 - \lambda} - \frac{|\xi_{\mathbf{m}}|^2}{|\xi_{\mathbf{m}}|^4 + 1} \right]$$

with a constant  $\alpha_0$  defined as

$$(4.5) \quad \alpha_0 = \lim_{\omega \rightarrow \infty} \left[ \frac{\ln \omega}{2\pi} - \frac{1}{|\Gamma|} \sum_{\substack{\mathbf{m} \in \mathbb{Z}^2 \\ |\xi_{\mathbf{m}}| \leq \omega}} \frac{|\xi_{\mathbf{m}}|^2}{|\xi_{\mathbf{m}}|^4 + 1} \right].$$

On the other hand, the unperturbed eigenvalues  $\lambda$  are given as the eigenvalues of  $-\Delta(\mathbf{k})$  with  $\text{mult}(\lambda, -\Delta(\mathbf{k})) > 1$ . More precisely, let  $\mu = \text{mult}(\lambda, -\Delta(\mathbf{k}))$ . Then there exist  $\mathbf{m}_1, \dots, \mathbf{m}_\mu \in \mathbb{Z}^2$  such that

$$\lambda = |\xi_{\mathbf{m}_1} + \mathbf{k}|^2 = \dots = |\xi_{\mathbf{m}_\mu} + \mathbf{k}|^2.$$

Then we have

$$(4.6) \quad \text{mult}(\lambda, -\Delta_{\alpha, \{\mathbf{0}\}}(\mathbf{k})) = \text{mult}(\lambda, -\Delta(\mathbf{k})) - 1$$

with the corresponding eigenspace

$$\left\{ f = \sum_{j=1}^{\mu} c_j e^{i(\xi_{\mathbf{m}_j} + \mathbf{k}) \cdot \bullet} \mid f(\mathbf{0}) = 0, c_1, \dots, c_\mu \in \mathbb{C} \right\}$$

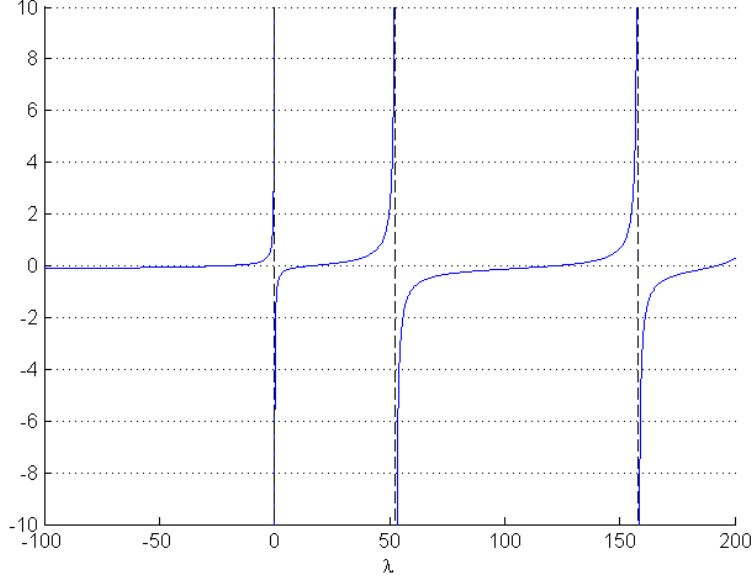


FIGURE 3. RHS of (4.3) when  $\mathbf{k} = (0, 0)$ . The dashed vertical lines represent  $\lambda \in \sigma(-\Delta(\mathbf{k}))$

In particular, if  $\text{mult}(\lambda, -\Delta(\mathbf{k})) = 1$ , then  $\lambda \notin \sigma(-\Delta_{\alpha, \{\mathbf{0}\}}(\mathbf{k}))$ .

The global properties of dispersion surfaces and spectral bands have been examined in [2] for rectangular two-dimensional lattices with one scatterer in each fundamental domain. Here we introduce an application to the triangular lattice  $\Lambda$ . The proof is similar to that of Theorem III.4.7 in [2].

**Proposition 4.2.** *Let  $\nu_1(\mathbf{k}, \alpha) \leq \nu_2(\mathbf{k}, \alpha) \leq \dots$  be the eigenvalues of  $-\Delta_{\alpha, \{\mathbf{0}\}}(\mathbf{k})$ . For  $\alpha \in \mathbb{R}$  and  $\beta = (\alpha, \alpha, \dots)$ , the spectrum of the operator  $-\Delta_{\beta, \Lambda}$  is purely absolutely continuous and equals*

$$(4.7) \quad \sigma(-\Delta_{\beta, \Lambda}) = [\nu_1(\alpha, \mathbf{0}), \nu_1(\alpha, \mathbf{K})] \cup [\nu_2(\alpha), \infty)$$

where

$$(4.8) \quad \nu_2(\alpha) = \min \left\{ \nu_2(\mathbf{0}, \alpha), \nu_2 \left( \frac{\mathbf{k}_1 + \mathbf{k}_2}{2}, \alpha \right) \right\} > 0 \quad \alpha \in \mathbb{R}$$

In addition,  $\alpha \mapsto \nu_j(\mathbf{k}, \alpha)$  is strictly increasing on  $\mathbb{R}$ , namely,

$$(4.9) \quad \frac{\partial \nu_j(\mathbf{k}, \alpha)}{\partial \alpha} > 0, \quad \alpha \in \mathbb{R}, \quad \mathbf{k} \in \mathcal{B}, \quad j = 1, 2, \dots$$

Hence, there exists  $\alpha_1$  such that

$$(4.10) \quad \sigma(-\Delta_{\beta, \Lambda}) = [\nu_1(\alpha, \mathbf{0}), \infty), \quad \alpha \geq \alpha_1$$

See Figure 4 and <http://math.berkeley.edu/~lmj0425/floq1dual.avi> for the global view of first five dispersion surfaces with various  $\alpha$ 's. See also Figure 5 for the graph of spectral bands  $\sigma(-\Delta_{\beta, \Lambda})$  versus  $\alpha$  where  $\beta = (\alpha, \alpha, \dots)$ .

On the other hand, we observe additional conic singularities of dispersion surfaces near Dirac point due to the symmetry property of the triangular lattice.



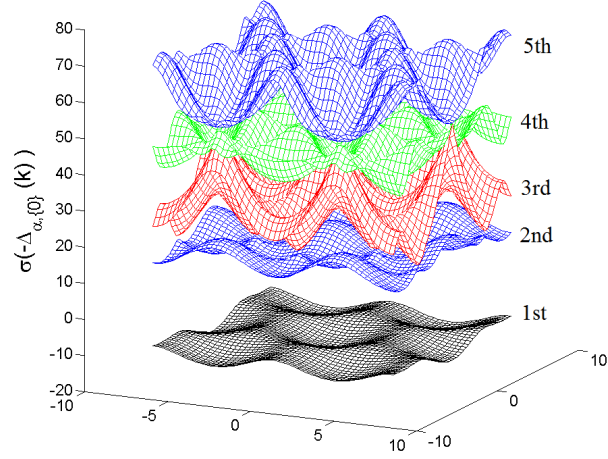


FIGURE 4. Global view of the first five dispersion surfaces generated by  $-\Delta_{0,\{0\}}(\mathbf{k})$ .

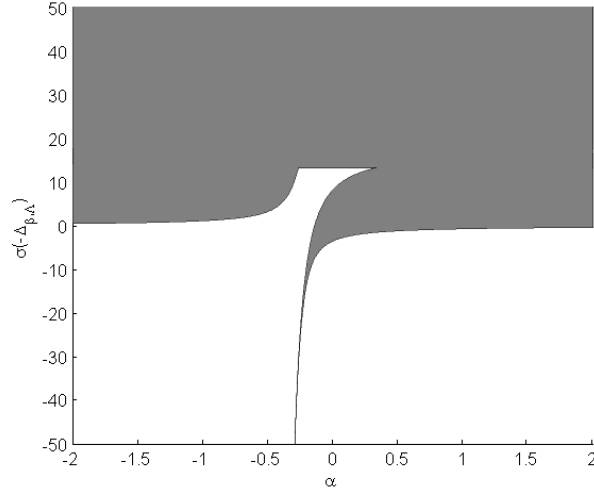


FIGURE 5. Spectrum of the triangular lattice point scatterer  $-\Delta_{\beta,\Lambda}$ ,  $\beta = (\alpha, \alpha, \dots)$  with respect to the coupling constant  $\alpha$ . The vertical section of the shaded region at each  $\alpha$  represents  $\sigma(-\Delta_{\beta,\Lambda})$ .

**Proposition 4.3.** As  $|\mathbf{k} - \mathbf{K}| \rightarrow 0$ ,

$$(4.11) \quad \nu_2(\mathbf{k}, \alpha) = |\mathbf{K}|^2 - \frac{4\pi}{3a}|\mathbf{k} - \mathbf{K}| + o(|\mathbf{k} - \mathbf{K}|)$$

$$(4.12) \quad \nu_3(\mathbf{k}, \alpha) = |\mathbf{K}|^2 + \frac{4\pi}{3a}|\mathbf{k} - \mathbf{K}| + o(|\mathbf{k} - \mathbf{K}|)$$

*Proof.* We have  $\nu_2(\mathbf{K}, \alpha) = \nu_3(\mathbf{K}, \alpha) = |\mathbf{K}|^2$  by (4.6), whereas  $\nu_1(\mathbf{K}, \alpha) < |\mathbf{K}|^2$  is obtained by (4.2). Consider  $\delta\mathbf{k}$  with  $|\delta\mathbf{k}| \ll 1$  such that  $|\mathbf{K} + \delta\mathbf{k}|$ ,  $|\mathbf{K} + R\delta\mathbf{k}|$ , and  $|\mathbf{K} + R^2\delta\mathbf{k}|$  have distinct values where  $R$  is defined by (4.1). Then we decompose

the direction vector  $\mathbf{u} = \frac{\delta \mathbf{k}}{|\delta \mathbf{k}|} \in \mathbb{S}^1$  into

$$\mathbf{u} = u_1 \frac{\mathbf{k}_1}{|\mathbf{k}_1|} + u_2 \frac{\mathbf{k}_2}{|\mathbf{k}_2|}$$

where

$$(4.13) \quad u_1^2 + u_2^2 - u_1 u_2 = 1.$$

and

$$(4.14) \quad |\mathbf{k}_1| = |\mathbf{k}_2| = \frac{4\pi}{a\sqrt{3}}.$$

Therefore,

$$(4.15) \quad \begin{aligned} |\mathbf{K} + \delta \mathbf{k}|^2 &= |\mathbf{K}|^2 + u_1 |\mathbf{k}_1| |\delta \mathbf{k}| + |\delta \mathbf{k}|^2 \\ |\mathbf{K} + R\delta \mathbf{k}|^2 &= |\mathbf{K}|^2 + (u_2 - u_1) |\mathbf{k}_1| |\delta \mathbf{k}| + |\delta \mathbf{k}|^2 \\ |\mathbf{K} + R^2\delta \mathbf{k}|^2 &= |\mathbf{K}|^2 - u_2 |\mathbf{k}_1| |\delta \mathbf{k}| + |\delta \mathbf{k}|^2 \end{aligned}$$

Suppose  $\lambda' = |\mathbf{K}|^2 + \delta\lambda$  solves (4.2) at  $\mathbf{k} = \mathbf{K} + \delta \mathbf{k}$ , namely,

$$(4.16) \quad |\Gamma|\alpha = \lim_{\omega \rightarrow \infty} \left[ \sum_{\substack{\mathbf{m} \in \mathbb{Z}^2 \\ |\xi_{\mathbf{m}} + \mathbf{K} + \delta \mathbf{k}| \leq \omega}} \frac{1}{|\xi_{\mathbf{m}} + \mathbf{K} + \delta \mathbf{k}|^2 - \lambda'} - \frac{2\pi}{|\mathcal{B}|} \ln \omega \right].$$

To simplify the notation, let  $\mathcal{M}_0 = \{\mathbf{m} \in \mathbb{Z}^2 \mid |\xi_{\mathbf{m}} + \mathbf{K}| = |\mathbf{K}|\} = \{(0, 0), (-1, 0), (-1, -1)\}$  and let

$$C_0 = \lim_{\omega \rightarrow \infty} \left[ \sum_{\substack{\mathbf{m} \in \mathbb{Z}^2 \setminus \mathcal{M}_0 \\ |\xi_{\mathbf{m}} + \mathbf{K}| \leq \omega}} \frac{1}{|\xi_{\mathbf{m}} + \mathbf{K}|^2 - \lambda'} - \frac{2\pi}{|\mathcal{B}|} \ln \omega \right]$$

Then due to the assumption on  $\delta \mathbf{k}$ , (4.16) reads

$$\begin{aligned} |\Gamma|\alpha - C_0 &= \frac{1}{|\mathbf{K} + \delta \mathbf{k}|^2 - \lambda'} + \frac{1}{|\xi_{(-1,0)} + \mathbf{K} + \delta \mathbf{k}|^2 - \lambda'} + \frac{1}{|\xi_{(-1,-1)} + \mathbf{K} + \delta \mathbf{k}|^2 - \lambda'} \\ &= \frac{1}{|\mathbf{K} + \delta \mathbf{k}|^2 - \lambda'} + \frac{1}{|\mathbf{K} + R\delta \mathbf{k}|^2 - \lambda'} + \frac{1}{|\mathbf{K} + R^2\delta \mathbf{k}|^2 - \lambda'} \\ &= \frac{1}{|\mathbf{k}_1| |\delta \mathbf{k}| u_1 - |\delta \mathbf{k}|^2 - \delta \lambda} + \frac{1}{|\mathbf{k}_1| |\delta \mathbf{k}| (-u_1 + u_2) - |\delta \mathbf{k}|^2 - \delta \lambda} \\ &\quad + \frac{1}{|\mathbf{k}_1| |\delta \mathbf{k}| (-u_2) - |\delta \mathbf{k}|^2 - \delta \lambda} \end{aligned}$$

Multiplying  $|\delta \mathbf{k}|$  on both sides, we obtain as  $|\delta \mathbf{k}| \rightarrow 0$ ,

$$\frac{1}{|\mathbf{k}_1| u_1 - \frac{\delta \lambda}{|\delta \mathbf{k}|}} + \frac{1}{|\mathbf{k}_1| (u_2 - u_1) - \frac{\delta \lambda}{|\delta \mathbf{k}|}} + \frac{1}{|\mathbf{k}_1| (-u_2) - \frac{\delta \lambda}{|\delta \mathbf{k}|}} \rightarrow 0$$

By (4.13) and (4.14),

$$\lim_{|\delta \mathbf{k}| \rightarrow 0} \frac{\delta \lambda}{\delta \mathbf{k}} = \pm \frac{|\mathbf{k}_1|}{\sqrt{3}} = \pm \frac{4\pi}{3a}$$

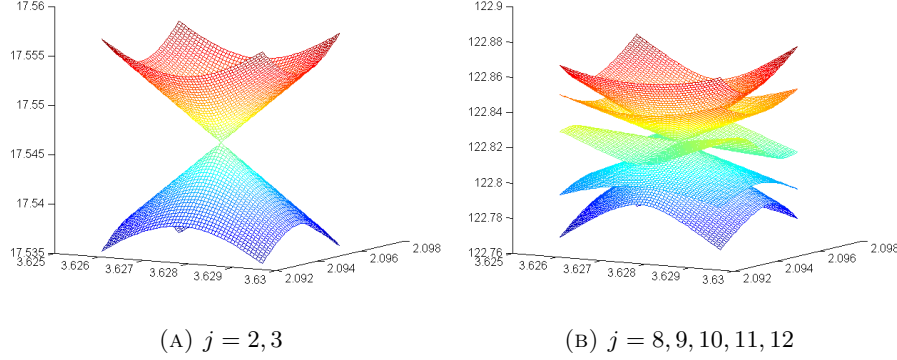


FIGURE 6. Local view of the  $j$ -th dispersion surface generated by  $-\Delta_{0,\{0\}}(\mathbf{k})$  near Dirac Point  $\mathbf{K}$ . See <http://math.berkeley.edu/~lmj0425/floq1dual.avi> for the first five dispersion surfaces where  $\alpha$  varies from 100 to  $-100$ .

By the continuity of dispersion surfaces, we can extend this result to any direction  $\mathbf{u} \in \mathbb{S}^1$ . So we obtain the directional derivative of  $\mathbf{k} \mapsto \nu_j(\mathbf{k}, \alpha)$  at  $\mathbf{k} = \mathbf{K}$ ,  $j = 2, 3$  as follows:

$$\nabla_{\mathbf{u}} \nu_2(\mathbf{K}, \alpha) = -\frac{4\pi}{3a}, \quad \nabla_{\mathbf{u}} \nu_3(\mathbf{K}, \alpha) = +\frac{4\pi}{3a}$$

□

*Remark.* Using the same argument as in Proposition 4.3, we observe infinitely many additional pairs of dispersion surfaces with a  $(3n-1)$ -fold conic singularity at each  $(\mathbf{K}, \lambda')$  where

$$\lambda' \in \{|\xi_{\mathbf{m}} + \mathbf{K}|^2 \mid \mathbf{m} \in \mathbb{Z}^2\} = \sigma(-\Delta(\mathbf{K}))$$

and

$$(4.17) \quad 3n = \#\{\mathbf{m} \in \mathbb{Z}^2 \mid |\xi_{\mathbf{m}} + \mathbf{K}| = \lambda'\}$$

Furthermore, these are the only conic singularities at Dirac point since all the other perturbed eigenvalues  $\lambda' \in \sigma(-\Delta_{\alpha,\{0\}}(\mathbf{K})) \setminus \sigma(-\Delta(\mathbf{K}))$  have multiplicity 1. Note that  $n \geq 1$  is an integer since for any  $\mathbf{m} \in \mathbb{Z}^2$ , we have

$$|\xi_{\mathbf{m}} + \mathbf{K}| = |\tilde{R}\xi_{\mathbf{m}} + \mathbf{K}| = |\tilde{R}^2\xi_{\mathbf{m}} + \mathbf{K}|$$

where  $\tilde{R} : \mathbb{R}^2 \rightarrow \mathbb{R}^2$  is a  $\frac{2\pi}{3}$ -rotation around a Dirac Point  $-\mathbf{K}$ . For instance, the  $j$ -th dispersion surfaces with  $j = 2, 3$  and  $j = 8, \dots, 12$  form a 2-fold and a 5-fold conic singularity, respectively. (See Figure 6.)

**4.2. Point scatterers on the honeycomb structure.** Consider the honeycomb structure defined in Section 2.

$$Y = \{0, \mathbf{x}_0\}, \quad \Lambda = \mathbb{Z}\mathbf{v}_1 \oplus \mathbb{Z}\mathbf{v}_2$$

Suppose the coupling constant for two scatterers at  $\mathbf{0}$  and  $\mathbf{x}_0$  are the same, say  $\alpha$ .

$$\boldsymbol{\alpha} = (\alpha, \alpha).$$

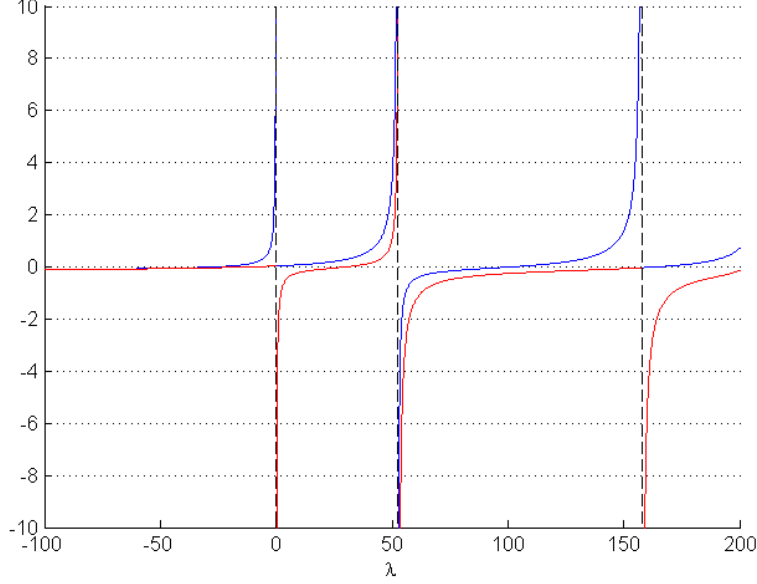


FIGURE 7. RHS of (4.18)(red) and (4.19)(blue), when  $\mathbf{k} = (0, 0)$ . The dashed vertical lines represent  $\lambda \in \sigma(-\Delta(\mathbf{k}))$

This is a legitimate assumption for the model of crystal structure which is comprised of only one element, such as carbon atoms in graphene. Then the set of perturbed eigenvalues,  $\sigma(-\Delta_{\alpha,Y}(\mathbf{k})) \setminus \sigma(-\Delta(\mathbf{k}))$ , is determined as follows:

**Proposition 4.4.** *Suppose  $\lambda' \notin \sigma(-\Delta(\mathbf{k}))$ . Then  $\lambda' \in \sigma(-\Delta_{\alpha,\{\mathbf{0},\mathbf{x}_0\}}(\mathbf{k}))$  if and only if*

$$(4.18) \quad \alpha = g_{\lambda'}(\mathbf{0}, \mathbf{k}) - |g_{\lambda'}(\mathbf{x}_0, \mathbf{k})|$$

or

$$(4.19) \quad \alpha = g_{\lambda'}(\mathbf{0}, \mathbf{k}) + |g_{\lambda'}(\mathbf{x}_0, \mathbf{k})|$$

In addition,

$$(4.20) \quad \text{mult}(\lambda', -\Delta_{\alpha,Y}(\mathbf{k})) = \dim \ker(\Gamma_{\alpha,\{\mathbf{0},\mathbf{x}_0\}}(\lambda', \mathbf{k}))$$

*Proof.* Suppose  $\lambda' \in \sigma(-\Delta_{\alpha,\{\mathbf{0},\mathbf{x}_0\}}(\mathbf{k})) \setminus \sigma(-\Delta(\mathbf{k}))$ . By (3.23),  $\Gamma_{\alpha,\{\mathbf{0},\mathbf{x}_0\}}(\lambda, \mathbf{k})$  is Hermitian for all  $\lambda \notin \sigma(-\Delta(\mathbf{k}))$ . So we can decompose  $\Gamma_{\alpha,\{\mathbf{0},\mathbf{x}_0\}}(\lambda, \mathbf{k})$  into

$$\Gamma_{\alpha,\{\mathbf{0},\mathbf{x}_0\}}(\lambda, \mathbf{k}) = U_{\alpha,\{\mathbf{0},\mathbf{x}_0\}}(\lambda, \mathbf{k}) \tilde{\Gamma}_{\alpha,\{\mathbf{0},\mathbf{x}_0\}}(\lambda, \mathbf{k}) U_{\alpha,\{\mathbf{0},\mathbf{x}_0\}}^*(\lambda, \mathbf{k})$$

where

$$(4.21) \quad U_{\alpha,\{\mathbf{0},\mathbf{x}_0\}}(\lambda, \mathbf{k}) = \begin{cases} \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & -\frac{g_{\lambda}(\mathbf{x}_0, \mathbf{k})}{|g_{\lambda}(\mathbf{x}_0, \mathbf{k})|} \\ \frac{\overline{g_{\lambda}(\mathbf{x}_0, \mathbf{k})}}{|g_{\lambda}(\mathbf{x}_0, \mathbf{k})|} & 1 \end{bmatrix} & \text{if } g_{\lambda}(\mathbf{x}_0, \mathbf{k}) \neq 0 \\ \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} & \text{if } g_{\lambda}(\mathbf{x}_0, \mathbf{k}) = 0 \end{cases}$$

and

$$(4.22) \quad \begin{aligned} \tilde{\Gamma}_{\alpha, \{\mathbf{0}, \mathbf{x}_0\}}(\lambda, \mathbf{k}) &= \text{diag}(\tilde{\gamma}_{1, \alpha, \{\mathbf{0}, \mathbf{x}_0\}}(\lambda, \mathbf{k}), \tilde{\gamma}_{2, \alpha, \{\mathbf{0}, \mathbf{x}_0\}}(\lambda, \mathbf{k})) \\ &= \text{diag}(\alpha - g_\lambda(\mathbf{0}, \mathbf{k}) + |g_\lambda(\mathbf{x}_0, \mathbf{k})|, \alpha - g_\lambda(\mathbf{0}, \mathbf{k}) - |g_\lambda(\mathbf{x}_0, \mathbf{k})|) \end{aligned}$$

Then for  $\lambda \notin \sigma(-\Delta_{\alpha, \{\mathbf{0}, \mathbf{x}_0\}}(\mathbf{k}))$ , we can rewrite (3.25) as

$$(4.23) \quad \begin{aligned} &(-\Delta_{\alpha, \{\mathbf{0}, \mathbf{x}_0\}}(\mathbf{k}) - \lambda)^{-1} f(\mathbf{x}) \\ &= (-\Delta(\mathbf{k}) - \lambda)^{-1} + \frac{1}{|\mathcal{B}|} \sum_{j=1}^N \tilde{\gamma}_{j, \alpha, \{\mathbf{0}, \mathbf{x}_0\}}^{-1}(\lambda, \mathbf{k}) \left( \overline{\tilde{g}_{j, \lambda}(\bullet, \mathbf{k})}, f \right) \tilde{g}_{j, \lambda}(\mathbf{x}, \mathbf{k}) \end{aligned}$$

where  $\tilde{g}_{j, \lambda}(\mathbf{x}, \mathbf{k})$  is the  $j$ -th entry of the vector

$$U_{\alpha, \{\mathbf{0}, \mathbf{x}_0\}}^*(\lambda, \mathbf{k}) \begin{bmatrix} g_\lambda(\mathbf{x}, \mathbf{k}) \\ g_\lambda(\mathbf{x} - \mathbf{x}_0, \mathbf{k}) \end{bmatrix}$$

In addition, we observe from (4.22) that

$$\partial_\lambda \tilde{\gamma}_{j, \alpha, \{\mathbf{0}, \mathbf{x}_0\}}(\lambda, \mathbf{k}) < 0, \quad j = 1, 2$$

which implies for  $\lambda' \in \sigma(-\Delta_{\alpha, \{\mathbf{0}, \mathbf{x}_0\}}(\mathbf{k})) \setminus \sigma(-\Delta(\mathbf{k}))$ ,

$$\tilde{\gamma}_{j, \alpha, \{\mathbf{0}, \mathbf{x}_0\}}(\lambda', \mathbf{k}) = 0 \quad \text{if and only if} \quad \text{Res}_{\lambda=\lambda'} \left( \tilde{\gamma}_{j, \alpha, \{\mathbf{0}, \mathbf{x}_0\}}^{-1}(\lambda, \mathbf{k}) \right) \neq 0, \quad j = 1, 2$$

So we obtain the multiplicity of  $\lambda = \lambda'$  as follows:

$$\begin{aligned} \text{mult}(\lambda', -\Delta_{\alpha, \{\mathbf{0}, \mathbf{x}_0\}}(\mathbf{k})) &= \text{rank} \oint_{\lambda'} (-\Delta_{\alpha, \{\mathbf{0}, \mathbf{x}_0\}}(\mathbf{k}) - \lambda)^{-1} d\lambda \\ &= \text{rank} \oint_{\lambda'} \frac{1}{|\mathcal{B}|} \sum_{j=1}^2 \tilde{\gamma}_{j, \alpha, \{\mathbf{0}, \mathbf{x}_0\}}^{-1}(\lambda, \mathbf{k}) \left( \overline{\tilde{g}_{j, \lambda}(\mathbf{k})}, \bullet \right) \tilde{g}_{j, \lambda}(\mathbf{k}) d\lambda \\ &= \# \left\{ j = 1, 2 \mid \text{Res}_{\lambda=\lambda'} \left( \tilde{\gamma}_{j, \alpha, \{\mathbf{0}, \mathbf{x}_0\}}^{-1}(\lambda, \mathbf{k}) \right) \neq 0 \right\} \\ &= \# \left\{ j = 1, 2 \mid \tilde{\gamma}_{j, \alpha, \{\mathbf{0}, \mathbf{x}_0\}}(\lambda', \mathbf{k}) = 0 \right\} \\ &= \dim \ker(\Gamma_{\alpha, \{\mathbf{0}, \mathbf{x}_0\}}(\lambda', \mathbf{k})) \end{aligned}$$

In addition, the corresponding eigenspace is the range of the operator:

$$(4.24) \quad \text{span} \left\{ \tilde{g}_{j, \lambda'}(\bullet, \mathbf{k}) \mid \tilde{\gamma}_{j, \alpha, \{\mathbf{0}, \mathbf{x}_0\}}(\lambda', \mathbf{k}) = 0, \quad j = 1, 2 \right\}$$

□

On the other hand, we observe that some eigenvalues of  $-\Delta(\mathbf{k})$  remain in the spectrum of  $-\Delta_{\alpha, \{\mathbf{0}, \mathbf{x}_0\}}(\mathbf{k})$  as unperturbed eigenvalues with multiplicity decreased by 0, 1 or 2.

**Proposition 4.5.** Suppose  $\lambda' = \lambda_{\mathbf{m}_1} = \dots = \lambda_{\mathbf{m}_\mu}$  is an eigenvalue of the unperturbed operator  $-\Delta(\mathbf{k})$  of multiplicity  $\mu$  where  $\lambda_{\mathbf{m}} = |\xi_{\mathbf{m}} + \mathbf{k}|^2$ . Then

$$(4.25) \quad \text{mult}(\lambda', -\Delta_{\alpha, \{\mathbf{0}, \mathbf{x}_0\}}(\mathbf{k})) = \begin{cases} \mu - 2 & \text{if } \mu \neq \left| \sum_{j=1}^{\mu} e^{i\xi_{\mathbf{m}_j} \cdot \mathbf{x}_0} \right| \quad (\text{Case 1}) \\ \mu - 1 & \text{if } \mu = \left| \sum_{j=1}^{\mu} e^{i\xi_{\mathbf{m}_j} \cdot \mathbf{x}_0} \right| \\ & \text{and } \alpha \neq \lim_{\lambda \nearrow \lambda'} (g_{\lambda}(\mathbf{0}, \mathbf{k}) - |g_{\lambda}(\mathbf{x}_0, \mathbf{k})|) \quad (\text{Case 2}) \\ \mu & \text{if } \mu = \left| \sum_{j=1}^{\mu} e^{i\xi_{\mathbf{m}_j} \cdot \mathbf{x}_0} \right| \\ & \text{and } \alpha = \lim_{\lambda \nearrow \lambda'} (g_{\lambda}(\mathbf{0}, \mathbf{k}) - |g_{\lambda}(\mathbf{x}_0, \mathbf{k})|) \quad (\text{Case 3}) \end{cases}$$

with the corresponding eigenspaces

(4.26)

$$(4.27) \quad (\text{Case 1}) \quad \left\{ f = \sum_{j=1}^{\mu} c_j e^{i(\xi_{\mathbf{m}_j} + \mathbf{k}) \cdot \bullet} \mid f(0) = f(\mathbf{x}_0) = 0, \ c_1, \dots, c_{\mu} \in \mathbb{C} \right\}$$

(4.28)

$$(4.28) \quad (\text{Case 2}) \quad \left\{ f = \sum_{j=1}^{\mu} c_j e^{i(\xi_{\mathbf{m}_j} + \mathbf{k}) \cdot \bullet} \mid f(0) = 0, \ c_1, \dots, c_{\mu} \in \mathbb{C} \right\}$$

(4.29)

$$(4.29) \quad (\text{Case 3}) \quad \left\{ f = \sum_{j=1}^{\mu} c_j e^{i(\xi_{\mathbf{m}_j} + \mathbf{k}) \cdot \bullet} \mid f(0) = 0, \ c_1, \dots, c_{\mu} \in \mathbb{C} \right\} \oplus \text{span} \left\{ \tilde{g}_{2, \lambda'}(\bullet, \mathbf{k}) \right\}$$

with  $\tilde{g}_{2, \lambda'}(\bullet, \mathbf{k}) = \lim_{\lambda \nearrow \lambda'} \tilde{g}_{2, \lambda}(\bullet, \mathbf{k})$  as in (4.24). Note that  $\text{mult}(\lambda', -\Delta_{\alpha, \{\mathbf{0}, \mathbf{x}_0\}}(\mathbf{k})) = 0$  means  $\lambda' \notin \sigma(-\Delta_{\alpha, \{\mathbf{0}, \mathbf{x}_0\}}(\mathbf{k}))$ .

*Proof.* First, consider the Laurent expansion of  $g_{\lambda}$  as  $\lambda \rightarrow \lambda'$ .

$$|\Gamma| g_{\lambda}(\mathbf{x}, \mathbf{k}) = - \sum_{j=1}^{\mu} e^{i\xi_{\mathbf{m}_j} \cdot \mathbf{x}_0} (\lambda - \lambda')^{-1} + R_{\lambda'}(\mathbf{x}, \mathbf{k}) + O(|\lambda - \lambda'|), \quad \lambda \rightarrow \lambda'$$

with the remainder term  $R_{\lambda}(\mathbf{x}, \mathbf{k}) = O(1)$ . Also, suppose  $f \in L_{\mathbf{k}}^2$  has the expansion

$$f(\mathbf{x}) = \sum_{\mathbf{m} \in \mathbb{Z}^2} f_{\mathbf{m}} e^{i(\xi_{\mathbf{m}} + \mathbf{k}) \cdot \mathbf{x}}, \quad f_{\mathbf{m}} = \frac{1}{|\mathcal{B}|} \int_{\mathcal{B}} f(\mathbf{x}) e^{-i(\xi_{\mathbf{m}} + \mathbf{k}) \cdot \mathbf{x}} d\mathbf{x}$$

Then we can rewrite the integral kernel of (3.25) for  $-\Delta_{\alpha, \{\mathbf{0}, \mathbf{x}_0\}}(\mathbf{k})$  using the matrix and vector notation.

$$(4.29) \quad (-\Delta_{\alpha, \{\mathbf{0}, \mathbf{x}_0\}}(\mathbf{k}) - \lambda)^{-1}(\mathbf{x}, \mathbf{x}') = g_{\lambda}(\mathbf{x} - \mathbf{x}') + \frac{1}{|\mathcal{B}|} [\vec{g}_{\lambda}(\mathbf{x}', \mathbf{k})]^T \left[ \frac{\text{adj } \Gamma_{\alpha, \{\mathbf{0}, \mathbf{x}_0\}}(\lambda, \mathbf{k})}{\det \Gamma_{\alpha, \{\mathbf{0}, \mathbf{x}_0\}}(\lambda, \mathbf{k})} \right] [\vec{g}_{\lambda}(\mathbf{x}, \mathbf{k})]$$

where each term has the Laurent expansion

$$\vec{g}_{\lambda}(\mathbf{x}, \mathbf{k}) = \begin{bmatrix} -\sum_{j=1}^{\mu} e^{i(\xi_{\mathbf{m}_j} + \mathbf{k}) \cdot \mathbf{x}} \\ -\sum_{j=1}^{\mu} e^{i(\xi_{\mathbf{m}_j} + \mathbf{k}) \cdot (\mathbf{x} - \mathbf{x}_0)} \end{bmatrix} (\lambda - \lambda')^{-1} + \begin{bmatrix} R_{\lambda'}(\mathbf{x}, \mathbf{k}) \\ R_{\lambda'}(\mathbf{x} - \mathbf{x}_0, \mathbf{k}) \end{bmatrix} + O(|\lambda - \lambda'|)$$

$$\begin{aligned} \text{adj } \Gamma_{\alpha, \{\mathbf{0}, \mathbf{x}_0\}}(\lambda, \mathbf{k}) &= \begin{bmatrix} \mu & -\sum_{j=1}^{\mu} e^{i(\xi_{\mathbf{m}_j} + \mathbf{k}) \cdot \mathbf{x}_0} \\ -\sum_{j=1}^{\mu} e^{-i(\xi_{\mathbf{m}_j} + \mathbf{k}) \cdot \mathbf{x}_0} & \mu \end{bmatrix} (\lambda - \lambda')^{-1} \\ &\quad + \begin{bmatrix} \alpha - R_{\lambda'}(\mathbf{0}, \mathbf{k}) & R_{\lambda'}(\mathbf{x}_0, \mathbf{k}) \\ R_{\lambda'}(-\mathbf{x}_0, \mathbf{k}) & \alpha - R_{\lambda'}(\mathbf{0}, \mathbf{k}) \end{bmatrix} + O(|\lambda - \lambda'|) \end{aligned}$$

$$\begin{aligned} \det \Gamma_{\alpha, \{\mathbf{0}, \mathbf{x}_0\}}(\lambda, \mathbf{k}) &= \left( \mu^2 - \left| \sum_{j=1}^{\mu} e^{i\xi_{\mathbf{m}_j} \cdot \mathbf{x}_0} \right|^2 \right) (\lambda - \lambda')^{-2} \\ &\quad + 2 \left( \mu(\alpha - R_{\lambda'}(\mathbf{0})) + \text{Re} \left( \sum_{j=1}^{\mu} e^{-i\xi_{\mathbf{m}_j} \cdot \mathbf{x}_0} R_{\lambda'}(\mathbf{x}_0) \right) \right) (\lambda - \lambda')^{-1} \\ &\quad + O(1) \\ &= C_{-2}(\lambda - \lambda')^{-2} + C_{-1}(\lambda - \lambda')^{-1} + C_0 + O(|\lambda - \lambda'|) \end{aligned}$$

*Case 1:* Suppose  $\mu \neq \left| \sum_{j=1}^{\mu} e^{i\xi_{\mathbf{m}_j} \cdot \mathbf{x}_0} \right|$ . Consider an operator  $P : L_{\mathbf{k}}^2 \rightarrow L_{\mathbf{k}}^2$  as the norm limit

$$P = \lim_{\lambda \rightarrow \lambda'} (\lambda - \lambda') (-\Delta_{\alpha, \{\mathbf{0}, \mathbf{x}_0\}}(\mathbf{k}) - \lambda)^{-1}$$

Then  $P$  is a projection onto the eigenspace corresponding to the eigenvalue  $\lambda = \lambda'$ . Since  $C_{-2} \neq 0$ , for all  $f \in L_{\mathbf{k}}^2$ ,

$$\begin{aligned} Pf(\mathbf{x}) &= \sum_{j=1}^{\mu} e^{i(\xi_{\mathbf{m}_j} + \mathbf{k}) \cdot \mathbf{x}} f_{\mathbf{m}_j} - \frac{1}{C_{-2}} \left[ \sum_{\mathbf{m}_j} f_{\mathbf{m}_j} \sum_{\mathbf{m}_j} e^{i(\xi_{\mathbf{m}_j} + \mathbf{k}) \cdot \mathbf{x}_0} \right]^T \\ &\quad \begin{bmatrix} \mu & -\sum_{\mathbf{m}_j} e^{i(\xi_{\mathbf{m}_j} + \mathbf{k}) \cdot \mathbf{x}_0} \\ -\sum_{\mathbf{m}_j} e^{-i(\xi_{\mathbf{m}_j} + \mathbf{k}) \cdot \mathbf{x}_0} & \mu \end{bmatrix} \begin{bmatrix} \sum_{\mathbf{m}_j} e^{i(\xi_{\mathbf{m}_j} + \mathbf{k}) \cdot \mathbf{x}} \\ \sum_{\mathbf{m}_j} e^{i(\xi_{\mathbf{m}_j} + \mathbf{k}) \cdot (\mathbf{x} - \mathbf{x}_0)} \end{bmatrix} \end{aligned}$$

Hence, we can show that  $P$  is the projection of  $f$  onto the eigenspace (4.26) since

$$Pf(\mathbf{0}) = 0, \quad Pf(\mathbf{x}_0) = 0$$

*Case 2:* Suppose  $\mu = \left| \sum_{j=1}^{\mu} e^{i\xi_{\mathbf{m}_j} \cdot \mathbf{x}_0} \right|$  and  $\alpha \neq \lim_{\lambda \nearrow \lambda'} (g_{\lambda}(\mathbf{0}, \mathbf{k}) - |g_{\lambda}(\mathbf{x}_0, \mathbf{k})|)$ . Since  $C_{-2} = 0$  and  $C_{-1} \neq 0$ ,

$$\begin{aligned} Pf(\mathbf{x}) &= \sum_{j=1}^{\mu} e^{i(\xi_{\mathbf{m}_j} + \mathbf{k}) \cdot \mathbf{x}} f_{\mathbf{m}_j} - \frac{1}{C_{-1}} \left( \sum_{\mathbf{m}_j} f_{\mathbf{m}_j} \right) \left[ e^{i(\xi_{\mathbf{m}_1} + \mathbf{k}) \cdot \mathbf{x}_0} \right]^T \\ &\quad \begin{bmatrix} \alpha - R_{\lambda'}(\mathbf{0}, \mathbf{k}) & R_{\lambda'}(\mathbf{x}_0, \mathbf{k}) \\ R_{\lambda'}(-\mathbf{x}_0, \mathbf{k}) & \alpha - R_{\lambda'}(\mathbf{0}, \mathbf{k}) \end{bmatrix} \begin{bmatrix} 1 \\ e^{-i(\xi_{\mathbf{m}_1} + \mathbf{k}) \cdot \mathbf{x}_0} \end{bmatrix} \left( \sum_{\mathbf{m}_j} e^{i(\xi_{\mathbf{m}_j} + \mathbf{k}) \cdot \mathbf{x}} \right) \\ &= \sum_{j=1}^{\mu} e^{i(\xi_{\mathbf{m}_j} + \mathbf{k}) \cdot \mathbf{x}} f_{\mathbf{m}_j} - \left( \sum_{j=1}^{\mu} f_{\mathbf{m}_j} \right) \left( \sum_{j=1}^{\mu} e^{i(\xi_{\mathbf{m}_j} + \mathbf{k}) \cdot \mathbf{x}} \right) \end{aligned}$$

Hence,  $P$  is the projection onto (4.27).

*Case 3:* Suppose  $\mu = \left| \sum_{j=1}^{\mu} e^{i\xi_{\mathbf{m}_j} \cdot \mathbf{x}_0} \right|$  and  $\alpha = \lim_{\lambda \nearrow \lambda'} (g_{\lambda}(\mathbf{0}, \mathbf{k}) - |g_{\lambda}(\mathbf{x}_0, \mathbf{k})|)$ . Since  $C_{-2} = 0$ ,  $C_{-1} = 0$  and  $C_0 \neq 0$ ,

$$\begin{aligned} Pf(\mathbf{x}) &= \sum_{j=1}^{\mu} e^{i(\xi_{\mathbf{m}_j} + \mathbf{k}) \cdot \mathbf{x}} f_{\mathbf{m}_j} - \frac{1}{C_0} \left[ \frac{(\overline{R_{\lambda'}}(\bullet, \mathbf{k}), f)}{(\overline{R_{\lambda'}}(\bullet - \mathbf{x}_0, \mathbf{k}), f)} \right]^T \\ &\quad \begin{bmatrix} \mu & -\sum_{j=1}^{\mu} e^{i(\xi_{\mathbf{m}_j} + \mathbf{k}) \cdot \mathbf{x}_0} \\ -\sum_{j=1}^{\mu} e^{-i(\xi_{\mathbf{m}_j} + \mathbf{k}) \cdot \mathbf{x}_0} & \mu \end{bmatrix} \begin{bmatrix} R_{\lambda'}(\mathbf{x}, \mathbf{k}) \\ R_{\lambda'}(\mathbf{x} - \mathbf{x}_0, \mathbf{k}) \end{bmatrix} \\ &\quad - \frac{1}{C_0} \left( \sum f_{\mathbf{m}_j} \right) \begin{bmatrix} 1 \\ e^{i(\xi_{\mathbf{m}_1} + \mathbf{k}) \cdot \mathbf{x}_0} \end{bmatrix}^T \begin{bmatrix} -R_{\lambda'}^2(\mathbf{0}) & R_{\lambda'}^2(\mathbf{x}_0) \\ -R_{\lambda'}^2(\mathbf{0}) & R_{\lambda'}^2(\mathbf{x}_0) \end{bmatrix} \\ &\quad \begin{bmatrix} 1 \\ e^{-i(\xi_{\mathbf{m}_1} + \mathbf{k}) \cdot \mathbf{x}_0} \end{bmatrix} \left( \sum e^{i(\xi_{\mathbf{m}_j} + \mathbf{k}) \cdot \mathbf{x}} \right) \\ &= \sum_{j=1}^{\mu} e^{i(\xi_{\mathbf{m}_j} + \mathbf{k}) \cdot \mathbf{x}} f_{\mathbf{m}_j} - \left( \sum_{j=1}^{\mu} f_{\mathbf{m}_j} \right) \left( \sum_{j=1}^{\mu} e^{i(\xi_{\mathbf{m}_j} + \mathbf{k}) \cdot \mathbf{x}} \right) \\ &\quad + C \left( \tilde{g}_{2, \lambda'}(\bullet, \mathbf{k}), f \right) \tilde{g}_{2, \lambda'}(\mathbf{x}, \mathbf{k}), \quad \text{for some } C \neq 0 \end{aligned}$$

Hence,  $P$  is the projection onto (4.28).  $\square$

*Remark.* Although the conditions for *Case 2* and *Case 3* seem restrictive in some sense, we can observe various cases satisfying those conditions. For example, suppose  $\mathbf{k} = (k_x, 0) \in \mathcal{B}$ ,  $k_x > 0$  and choose  $\lambda'$  as

$$\lambda' = |\xi_{(0, -1)} + \mathbf{k}| = |\xi_{(-1, 0)} + \mathbf{k}|$$

so that  $\lambda'$  is an eigenvalue of  $-\Delta(\mathbf{k})$  of multiplicity  $\mu = 2$ . Then we have

$$\left| e^{i\xi_{(0, -1)} \cdot \mathbf{x}_0} + e^{i\xi_{(-1, 0)} \cdot \mathbf{x}_0} \right| = \left| 2e^{-i\frac{4\pi}{3}} \right| = 2,$$

which falls into either *Case 2* or *Case 3* of (4.25) depending on the value of  $\alpha$ . Hence,

$$\text{mult}(\lambda', -\Delta_{\alpha, \{\mathbf{0}, \mathbf{x}_0\}}(\mathbf{k})) = \begin{cases} 1 & \text{if } \alpha \neq \lim_{\lambda \nearrow \lambda'} (g_{\lambda}(\mathbf{0}, \mathbf{k}) - |g_{\lambda}(\mathbf{x}_0, \mathbf{k})|) \\ 2 & \text{if } \alpha = \lim_{\lambda \nearrow \lambda'} (g_{\lambda}(\mathbf{0}, \mathbf{k}) - |g_{\lambda}(\mathbf{x}_0, \mathbf{k})|) \end{cases}.$$

On the other hand, suppose  $\mathbf{k} = (0, k_y) \in \mathcal{B}$ ,  $k_y > 0$  and choose  $\lambda'$  as

$$\lambda' = |\xi_{(0, 1)} + \mathbf{k}| = |\xi_{(-1, 0)} + \mathbf{k}|.$$

so that  $\mu = 2$ . Then we observe

$$\left| e^{i\xi_{(0, 1)} \cdot \mathbf{x}_0} + e^{i\xi_{(-1, 0)} \cdot \mathbf{x}_0} \right| = \left| e^{i\frac{4\pi}{3}} + e^{-i\frac{4\pi}{3}} \right| \neq 2,$$

which corresponds to *Case 1* of (4.25). Therefore,  $\text{mult}(\lambda', -\Delta_{\alpha, \{\mathbf{0}, \mathbf{x}_0\}}(\mathbf{k})) = 0$ , which implies

$$\lambda' \notin \sigma(-\Delta_{\alpha, \{\mathbf{0}, \mathbf{x}_0\}}(\mathbf{k})), \quad \alpha \in \mathbb{R}.$$

*Remark.* If  $\text{mult}(\lambda, -\Delta(\mathbf{k})) = 1$ , then  $\left| \sum_{j=1}^{\mu} e^{i\xi_{\mathbf{m}_j} \cdot \mathbf{x}_0} \right| = |e^{i\xi_{\mathbf{m}_1} \cdot \mathbf{x}_0}| = 1$  so this falls into either *Case 2* or *Case 3*.

$$\begin{cases} \lambda \notin \sigma(-\Delta_{\alpha, \{\mathbf{0}, \mathbf{x}_0\}}(\mathbf{k})) & \text{if } \alpha \neq \lim_{\lambda \nearrow \lambda'} (g_{\lambda}(\mathbf{0}, \mathbf{k}) - |g_{\lambda}(\mathbf{x}_0, \mathbf{k})|) \\ \lambda \in \sigma(-\Delta_{\alpha, \{\mathbf{0}, \mathbf{x}_0\}}(\mathbf{k})) & \text{if } \alpha = \lim_{\lambda \nearrow \lambda'} (g_{\lambda}(\mathbf{0}, \mathbf{k}) - |g_{\lambda}(\mathbf{x}_0, \mathbf{k})|) \end{cases}$$



On the other hand, if  $\text{mult}(\lambda, -\Delta(\mathbf{k})) \geq 3$ , then

$$\lambda \in \sigma(-\Delta_{\alpha, \{0, \mathbf{x}_0\}}(\mathbf{k})).$$

Also, we can easily show that the dispersion surfaces  $\lambda_1(\mathbf{k}, \alpha) \leq \lambda_2(\mathbf{k}, \alpha) \leq \dots$  given as functions of  $\mathbf{k}$  by Theorem 4.4 and Theorem 4.5 are continuous and  $\mathcal{B}$ -periodic so they are literally "surfaces" over the Brillouin Zone. Now consider the spectrum as a function of the coupling constant  $\alpha$ . Note that  $\alpha = \infty$  corresponds to the free Hamiltonian  $-\Delta(\mathbf{k})$ .

**Theorem 4.6.** *Let  $\lambda_1(\mathbf{k}, \alpha) \leq \lambda_2(\mathbf{k}, \alpha) \leq \dots$  and  $\lambda_1^\infty(\mathbf{k}) \leq \lambda_2^\infty(\mathbf{k}) \leq \dots$  be the eigenvalues of  $\sigma(-\Delta_{\alpha, \{0, \mathbf{x}_0\}}(\mathbf{k}))$  and  $\sigma(-\Delta(\mathbf{k}))$ , respectively. Then  $\alpha \mapsto \lambda_j(\mathbf{k}, \alpha)$  is increasing for all  $j$  and*

$$\lambda_j(\mathbf{k}, \alpha) \geq \lambda_1^\infty(\mathbf{k}) \geq 0, \quad j \geq 3, \quad \forall \alpha$$

$$\lambda_j(\mathbf{k}, \alpha) \rightarrow -\infty \text{ as } \alpha \rightarrow -\infty \quad j = 1, 2$$

In addition,

$$\lim_{\alpha \rightarrow \infty} \lambda_j(\mathbf{k}, \alpha) = \lim_{\alpha \rightarrow -\infty} \lambda_{j+2}(\mathbf{k}, \alpha) = \lambda_j^\infty(\mathbf{k}) \quad \text{for all } j \geq 1$$

*Proof.* First,  $\lambda \mapsto g_\lambda(\mathbf{0}, \mathbf{k}) \pm |g_\lambda(\mathbf{x}_0, \mathbf{k})|$  is continuous and increasing for both signs for  $\lambda \in (-\infty, \lambda_1^\infty(\mathbf{k}))$ . In addition, we observe that

$$\lim_{\lambda \rightarrow -\infty} g_\lambda(\mathbf{0}, \mathbf{k}) \pm |g_\lambda(\mathbf{x}_0, \mathbf{k})| = -\infty$$

Therefore, by (4.18) and (4.19), there exist exactly two perturbed eigenvalues  $\lambda_1(\mathbf{k}, \alpha)$  and  $\lambda_2(\mathbf{k}, \alpha)$  in  $(-\infty, \lambda_1^\infty(\mathbf{k}))$  whenever

$$\alpha \leq \lim_{\lambda \nearrow \lambda_1^\infty(\mathbf{k})} (g_\lambda(\mathbf{0}, \mathbf{k}) - |g_\lambda(\mathbf{x}_0, \mathbf{k})|).$$

This also implies that

$$\lim_{\alpha \rightarrow -\infty} \lambda_j(\mathbf{k}, \alpha) \rightarrow -\infty, \quad j = 1, 2$$

On the other hand, consider the other eigenvalues near an arbitrary  $\lambda' \in \sigma(-\Delta(\mathbf{k}))$ . Since  $g_\lambda(\mathbf{0}, \mathbf{k}) \pm |g_\lambda(\mathbf{x}_0, \mathbf{k})|$  is finite for  $\lambda \notin \sigma(-\Delta(\mathbf{k}))$ , we observe that

$$\begin{cases} \lim_{\alpha \rightarrow \infty} \lambda_j(\mathbf{k}, \alpha) & \in \sigma(-\Delta(\mathbf{k})) \\ \lim_{\alpha \rightarrow -\infty} \lambda_{j+2}(\mathbf{k}, \alpha) & \in \sigma(-\Delta(\mathbf{k})) \end{cases} \quad \text{for all } j \geq 1$$

Therefore, it suffices to show that those two limits agree with the same multiplicity at  $\lambda = \lambda'$  for all  $j \geq 1$ . Note that as  $\lambda \rightarrow \lambda'$ ,

$$\begin{aligned} g_\lambda(\mathbf{0}, \mathbf{k}) &= -\frac{\mu}{|\Gamma|}(\lambda - \lambda')^{-1} + O(1) \\ |g_\lambda(\mathbf{x}_0, \mathbf{k})| &= \frac{1}{|\Gamma|} \left| \sum_{j=1}^{\mu} e^{i\xi_{\mathbf{m}_j} \cdot \mathbf{x}_0} \right| |\lambda - \lambda'|^{-1} + O(1) \end{aligned}$$

We consider two cases as follows:

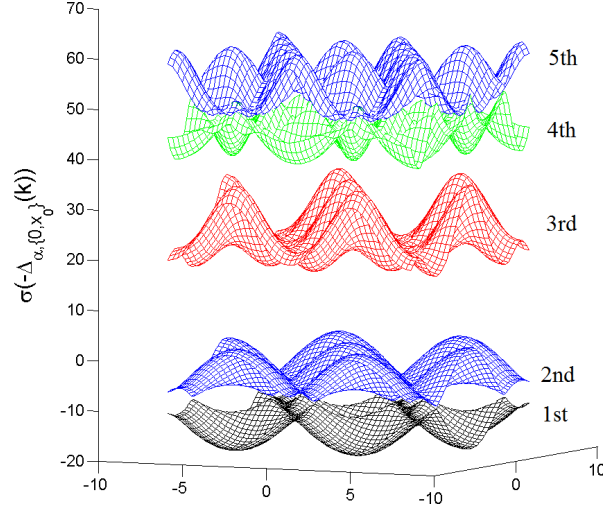


FIGURE 8. Global view of the first five dispersion surfaces generated by  $-\Delta_{\alpha, \{0, \mathbf{x}_0\}}(\mathbf{k})$ ,  $\alpha = -0.2$ .

*Case 1:* If  $\mu \neq \left| \sum_{j=1}^{\mu} e^{i\xi_{m_j} \cdot \mathbf{x}_0} \right|$  then the unperturbed eigenvalue  $\lambda = \lambda'$  loses its multiplicity by 2 according to Theorem 4.5. However, we also observe

$$\begin{cases} \lim_{\lambda \nearrow \lambda'} g_{\lambda}(\mathbf{0}, \mathbf{k}) + |g_{\lambda}(\mathbf{x}_0, \mathbf{k})| = \infty \\ \lim_{\lambda \nearrow \lambda'} g_{\lambda}(\mathbf{0}, \mathbf{k}) - |g_{\lambda}(\mathbf{x}_0, \mathbf{k})| = \infty \\ \lim_{\lambda \searrow \lambda'} g_{\lambda}(\mathbf{0}, \mathbf{k}) + |g_{\lambda}(\mathbf{x}_0, \mathbf{k})| = \infty \\ \lim_{\lambda \searrow \lambda'} g_{\lambda}(\mathbf{0}, \mathbf{k}) - |g_{\lambda}(\mathbf{x}_0, \mathbf{k})| = -\infty \end{cases}$$

which imply by Theorem 4.4 that there exists exactly two perturbed eigenvalues converging to  $\lambda = \lambda'$  as  $\alpha \rightarrow \pm\infty$ . So the multiplicity of  $\lambda = \lambda'$  is conserved for both cases when  $\alpha = +\infty$  and  $\alpha = -\infty$ .

*Case 2:* If  $\mu = \left| \sum_{j=1}^{\mu} e^{i\xi_{m_j} \cdot \mathbf{x}_0} \right|$  then the unperturbed eigenvalue  $\lambda = \lambda'$  loses its multiplicity by 1 for  $|\alpha|$  sufficiently large according to Theorem 4.5. However, we also observe

$$\begin{cases} \lim_{\lambda \nearrow \lambda'} g_{\lambda}(\mathbf{0}, \mathbf{k}) + |g_{\lambda}(\mathbf{x}_0, \mathbf{k})| = \infty \\ \lim_{\lambda \nearrow \lambda'} g_{\lambda}(\mathbf{0}, \mathbf{k}) - |g_{\lambda}(\mathbf{x}_0, \mathbf{k})| = C \\ \lim_{\lambda \searrow \lambda'} g_{\lambda}(\mathbf{0}, \mathbf{k}) + |g_{\lambda}(\mathbf{x}_0, \mathbf{k})| = C \\ \lim_{\lambda \searrow \lambda'} g_{\lambda}(\mathbf{0}, \mathbf{k}) - |g_{\lambda}(\mathbf{x}_0, \mathbf{k})| = -\infty \end{cases}, \quad C \text{ is finite}$$

which imply by Theorem 4.4 that there exists exactly one perturbed eigenvalue converging to  $\lambda = \lambda'$  as  $\alpha \rightarrow \pm\infty$ . So the multiplicity of  $\lambda = \lambda'$  is conserved for both cases  $\alpha = +\infty$  and  $\alpha = -\infty$ .

This concludes the proof.  $\square$

4.2.1. *Eigenvalues near Dirac points.* Dirac Points in the dual lattice are located at the vertices of the Brillouin Zone boundary. (See Figure 2.) Without loss of generality we choose one Dirac point

$$\mathbf{K} = \frac{2}{3}\mathbf{k}_1 + \frac{1}{3}\mathbf{k}_2$$

and observe the conic dispersion surfaces generated by  $-\Delta_{\alpha, \{0, \mathbf{x}_0\}}(\mathbf{k})$  near  $\mathbf{k} = \mathbf{K}$ .

**Proposition 4.7.** *At Dirac point  $\mathbf{K}$ , the perturbed eigenvalues of  $-\Delta_{\alpha, \{0, \mathbf{x}_0\}}(\mathbf{K})$  has multiplicity 2 and coincides with those of the triangular lattice operator  $-\Delta_{\alpha, \{0\}}(\mathbf{K})$ , namely,*

$$\sigma(-\Delta_{\alpha, \{0, \mathbf{x}_0\}}(\mathbf{K})) \setminus \sigma(-\Delta(\mathbf{K})) = \sigma(-\Delta_{\alpha, \{0\}}(\mathbf{K})) \setminus \sigma(-\Delta(\mathbf{K}))$$

and for all  $\lambda' \in \sigma(-\Delta_{\alpha, \{0, \mathbf{x}_0\}}(\mathbf{K})) \setminus \sigma(-\Delta(\mathbf{K}))$ ,

$$\text{mult}(\lambda', -\Delta_{\alpha, \{0, \mathbf{x}_0\}}(\mathbf{K})) = 2$$

*Proof.* We use the symmetry of the honeycomb structure and dual lattice as in Section 2.4 of [1]. Let  $\tilde{R} : \mathbb{R}^2 \rightarrow \mathbb{R}^2$  be a  $\frac{2\pi}{3}$ -rotation around a Dirac Point  $-\mathbf{K}$ . Then we see

$$\begin{aligned} \tilde{R}\xi_{\mathbf{m}} &= \tilde{R}\xi_{(m_1, m_2)} = \xi_{(-m_1+m_2-1, -m_1-1)} \\ \tilde{R}^2\xi_{\mathbf{m}} &= \tilde{R}^2\xi_{(m_1, m_2)} = \xi_{(-m_2-1, m_1-m_2)} \\ \tilde{R}^3\xi_{\mathbf{m}} &= \text{Id } \xi_{(m_1, m_2)} = \xi_{(m_1, m_2)} \end{aligned} \tag{4.30}$$

Here we abuse the notation and write  $\tilde{R}\xi_{\mathbf{m}} = \xi_{\tilde{R}\mathbf{m}}$  so that

$$\begin{aligned} \tilde{R}\mathbf{m} &= \tilde{R}(m_1, m_2) = (-m_1 + m_2 - 1, -m_1 - 1) \\ \tilde{R}^2\mathbf{m} &= \tilde{R}^2(m_1, m_2) = (-m_2 - 1, m_1 - m_2) \\ \tilde{R}^3\mathbf{m} &= \text{Id } (m_1, m_2) = (m_1, m_2) \end{aligned}$$

So we can decompose  $\mathbb{Z}^2$  into three disjoint subsets  $\mathcal{S}$ ,  $\tilde{R}\mathcal{S}$ , and  $\tilde{R}^2\mathcal{S}$  where

$$\mathbb{Z}^2 = \mathcal{S} \cup \tilde{R}\mathcal{S} \cup \tilde{R}^2\mathcal{S}$$

For instance,  $\{(0, 0), (-1, -1), (-1, 0)\}$  is an orbit of  $\tilde{R}$ . So we choose exactly one of them, say  $(0, 0)$ , as an element of  $\mathcal{S}$ . (See Definition 2.4 of [1].)

Since  $\mathbf{x}_0 = \frac{2}{3}(\mathbf{v}_1 + \mathbf{v}_2)$ , we obtain

$$\begin{aligned} \xi_{\mathbf{m}} \cdot \mathbf{x}_0 &= \frac{2\pi}{3}(m_1 + m_2) \\ \xi_{\tilde{R}\mathbf{m}} \cdot \mathbf{x}_0 &= \frac{2\pi}{3}(-2m_1 + m_2 - 2) = \frac{2\pi}{3}(m_1 + m_2) - (2\pi m_1 + \frac{4\pi}{3}) \\ \xi_{\tilde{R}^2\mathbf{m}} \cdot \mathbf{x}_0 &= \frac{2\pi}{3}(m_1 - 2m_2 - 1) = \frac{2\pi}{3}(m_1 + m_2) - (2\pi m_2 + \frac{2\pi}{3}) \end{aligned}$$

Therefore,

$$e^{i\xi_{\mathbf{m}} \cdot \mathbf{x}_0} + e^{i\xi_{\tilde{R}\mathbf{m}} \cdot \mathbf{x}_0} + e^{i\xi_{\tilde{R}^2\mathbf{m}} \cdot \mathbf{x}_0} = e^{i\frac{2\pi}{3}(m_1+m_2)} \left(1 + e^{i\frac{2\pi}{3}} + e^{i\frac{4\pi}{3}}\right) = 0$$

In addition, note that

$$|\xi_{\mathbf{m}} + \mathbf{K}| = |\xi_{\tilde{R}\mathbf{m}} + \mathbf{K}| = |\xi_{\tilde{R}^2\mathbf{m}} + \mathbf{K}|$$

Therefore, we can conclude that

$$\begin{aligned}
g_{\lambda'}(\mathbf{x}_0, \mathbf{K}) &= \sum_{\mathbf{m} \in \mathbb{Z}^2} \frac{e^{i\xi_{\mathbf{m}} \cdot \mathbf{x}_0}}{|\xi_{\mathbf{m}}^2 + \mathbf{K}|^2 - \lambda'} \\
&= \sum_{\mathbf{m} \in \mathcal{S}} \left[ \frac{e^{i\xi_{\mathbf{m}} \cdot \mathbf{x}_0}}{|\xi_{\mathbf{m}}^2 + \mathbf{K}|^2 - \lambda'} + \frac{e^{i\xi_{\tilde{R}\mathbf{m}} \cdot \mathbf{x}_0}}{|\xi_{\tilde{R}\mathbf{m}}^2 + \mathbf{K}|^2 - \lambda'} + \frac{e^{i\xi_{\tilde{R}^2\mathbf{m}} \cdot \mathbf{x}_0}}{|\xi_{\tilde{R}^2\mathbf{m}}^2 + \mathbf{K}|^2 - \lambda'} \right] \\
&= \sum_{\mathbf{m} \in \mathcal{S}} \frac{e^{i\xi_{\mathbf{m}} \cdot \mathbf{x}_0} + e^{i\xi_{\tilde{R}\mathbf{m}} \cdot \mathbf{x}_0} + e^{i\xi_{\tilde{R}^2\mathbf{m}} \cdot \mathbf{x}_0}}{|\xi_{\mathbf{m}}^2 + \mathbf{K}|^2 - \lambda'} \\
&= 0
\end{aligned}$$

Hence, (4.18) and (4.19) become two identical formulae and

$$\text{mult}(\lambda', -\Delta_{\alpha, \{0, \mathbf{x}_0\}}(\mathbf{K})) = 2 \quad \forall \lambda' \in \sigma(-\Delta_{\alpha, \{0, \mathbf{x}_0\}}(\mathbf{K})) \setminus \sigma(-\Delta(\mathbf{K}))$$

Moreover, (4.18) and (4.19) coincide with (4.3) of the triangular lattice case. Hence,

$$\sigma(-\Delta_{\alpha, \{0, \mathbf{x}_0\}}(\mathbf{K})) \setminus \sigma(-\Delta(\mathbf{K})) = \sigma(-\Delta_{\alpha, \{0\}}(\mathbf{K})) \setminus \sigma(-\Delta(\mathbf{K}))$$

□

In addition, those eigenvalues of multiplicity 2 given in the previous proposition are the conic points on the dispersion surfaces.

**Lemma 4.8.** *For each  $\lambda' \in \sigma(-\Delta_{\alpha, \{0, \mathbf{x}_0\}}(\mathbf{K})) \setminus \sigma(-\Delta(\mathbf{K}))$ , there exist two dispersion surfaces  $\mathbf{k} \mapsto \lambda_-(\mathbf{k})$  and  $\mathbf{k} \mapsto \lambda_+(\mathbf{k})$  of the operator  $-\Delta_{\alpha, \{0, \mathbf{x}_0\}}(\mathbf{k})$  such that  $\lambda' = \lambda_-(\mathbf{K}) = \lambda_+(\mathbf{K})$ . In addition,  $\lambda_+$  and  $\lambda_-$  meet conically at  $(\mathbf{K}, \lambda')$  with the directional derivatives independent of the direction  $\mathbf{u} \in \mathbb{S}^1$ ,*

$$\nabla_{\mathbf{u}} \lambda_{\pm}(\mathbf{K}) = \pm c(\lambda')$$

where  $c(\lambda') > 0$  is defined by

$$(4.31) \quad c(\lambda') = \frac{4\pi}{a} \frac{\left| \sum_{\mathbf{m} \in \mathbb{Z}^2} \frac{m_1 e^{i\xi_{\mathbf{m}} \cdot \mathbf{x}_0}}{(|\xi_{\mathbf{m}} + \mathbf{K}|^2 - \lambda')^2} \right|}{\sum_{\mathbf{m} \in \mathbb{Z}^2} \frac{1}{(|\xi_{\mathbf{m}} + \mathbf{K}|^2 - \lambda')^2}}, \quad \mathbf{m} = (m_1, m_2)$$

*Proof.* Suppose  $\lambda' \in \sigma(-\Delta_{\alpha, \{0, \mathbf{x}_0\}}(\mathbf{K})) \setminus \sigma(-\Delta(\mathbf{K}))$ . By Proposition 4.7,  $\lambda'$  is an eigenvalue of  $-\Delta_{\alpha, \{0, \mathbf{x}_0\}}(\mathbf{K})$  of multiplicity 2. So we can choose  $j$  such that  $\lambda' = \lambda_j(\mathbf{K}, \alpha) = \lambda_{j+1}(\mathbf{K}, \alpha)$ . Since  $\alpha$  is fixed, let

$$\lambda_+(\mathbf{k}) = \lambda_{j+1}(\mathbf{k}, \alpha)$$

$$\lambda_-(\mathbf{k}) = \lambda_j(\mathbf{k}, \alpha)$$

Now we prove the conic behavior of  $\mathbf{k} \mapsto \lambda_+(\mathbf{k})$  near  $\lambda = \lambda'$ . Consider a small perturbation  $\delta\mathbf{k}$  and the corresponding  $\delta\lambda$ :

$$\delta\mathbf{k} = |\delta\mathbf{k}|\mathbf{u} \in \mathbb{R}^2, \quad |\delta\mathbf{k}| \ll 1, \quad \mathbf{u} \in \mathbb{S}^1$$

$$\delta\lambda = \lambda_+(\mathbf{K} + \delta\mathbf{k}) - \lambda_+(\mathbf{K})$$

Then both  $(\mathbf{K}, \lambda')$  and  $(\mathbf{K} + \delta\mathbf{k}, \lambda' + \delta\lambda)$  solve (4.18):

$$(4.32) \quad \alpha - g_{\lambda'}(\mathbf{0}, \mathbf{K}) + |g_{\lambda'}(\mathbf{x}_0, \mathbf{K})| = 0$$

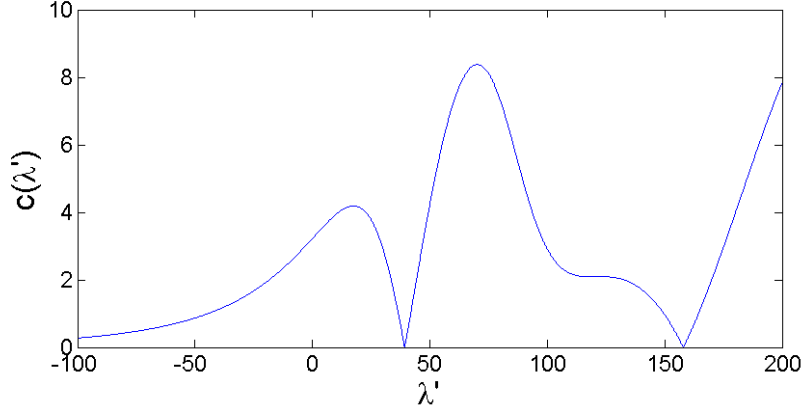


FIGURE 9. The directional derivative  $c(\lambda')$  of the conic surface at Dirac Point  $\mathbf{K}$  defined by (4.31) as a function of  $\lambda'$  when  $a = 1$ .

and

$$(4.33) \quad \alpha - g_{\lambda'+\delta\lambda}(\mathbf{0}, \mathbf{K} + \delta\mathbf{k}) + |g_{\lambda'+\delta\lambda}(\mathbf{x}_0, \mathbf{K} + \delta\mathbf{k})| = 0$$

Subtracting (4.32) from (4.33), we obtain

$$(4.34) \quad \sum_{m \in \mathbb{Z}^2} \frac{2(\xi_m + \mathbf{K}) \cdot \delta\mathbf{k} - \delta\lambda}{(|\xi_m + \mathbf{K}|^2 - \lambda')^2} + \left| \sum_{m \in \mathbb{Z}^2} \frac{e^{i\xi_m \cdot \mathbf{x}_0} (2(\xi_m + \mathbf{K}) \cdot \delta\mathbf{k} - \delta\lambda)}{(|\xi_m + \mathbf{K}|^2 - \lambda')^2} \right| = o(|\delta\mathbf{k}|)$$

In addition, we observe that

$$\sum_{m \in \mathbb{Z}^2} \frac{e^{i\xi_m \cdot \mathbf{x}_0}}{(|\xi_m + \mathbf{K}|^2 - \lambda')^2} = 0$$

and

$$\sum_{m \in \mathbb{Z}^2} \frac{\xi_m + \mathbf{K}}{(|\xi_m + \mathbf{K}|^2 - \lambda')^2} = \mathbf{0}$$

due to the symmetry property as in Proposition 4.7. So we can simplify (4.34) as

$$- \sum_{m \in \mathbb{Z}^2} \frac{\delta\lambda}{(|\xi_m + \mathbf{K}|^2 - \lambda')^2} + \left| \sum_{m \in \mathbb{Z}^2} 2 \frac{e^{i\xi_m \cdot \mathbf{x}_0} (\xi_m + \mathbf{K}) \cdot \delta\mathbf{k}}{(|\xi_m + \mathbf{K}|^2 - \lambda')^2} \right| = o(|\delta\mathbf{k}|)$$

Hence, as  $|\delta\mathbf{k}| \rightarrow 0$ , we obtain the directional derivative of the upper dispersion surface,

$$\nabla_{\mathbf{u}} \lambda_+(\mathbf{K}) = + \frac{\left| \sum_{m \in \mathbb{Z}^2} \frac{2e^{i\xi_m \cdot \mathbf{x}_0} (\xi_m + \mathbf{K})}{(|\xi_m + \mathbf{K}|^2 - \lambda')^2} \cdot \mathbf{u} \right|}{\sum_{m \in \mathbb{Z}^2} \frac{1}{(|\xi_m + \mathbf{K}|^2 - \lambda')^2}}$$

Define  $\mathbf{c} : \mathbb{R} \rightarrow \mathbb{C}^2$  by

$$\mathbf{c}(\lambda') = \frac{\sum_{m \in \mathbb{Z}^2} \frac{2e^{i\xi_m \cdot \mathbf{x}_0} (\xi_m + \mathbf{K})}{(|\xi_m + \mathbf{K}|^2 - \lambda')^2}}{\sum_{m \in \mathbb{Z}^2} \frac{1}{(|\xi_m + \mathbf{K}|^2 - \lambda')^2}}.$$

so that

$$\nabla_{\mathbf{u}} \lambda_+(\mathbf{K}) = |\mathbf{c}(\lambda') \cdot \mathbf{u}|$$

Then we observe that

$$e^{i\frac{\pi}{3}} \mathbf{c}(\lambda') \cdot \frac{\mathbf{v}_1}{a} = \mathbf{c}(\lambda') \cdot \frac{\mathbf{v}_2}{a}$$

which implies for any  $\mathbf{u} \in \mathbb{S}^1$ ,

$$\begin{aligned} |\mathbf{c}(\lambda') \cdot \mathbf{u}| &= \left| \mathbf{c}(\lambda') \cdot \frac{\mathbf{v}_1}{a} \right| \\ &= \frac{4\pi}{a} \frac{\left| \sum_{\mathbf{m} \in \mathbb{Z}^2} \frac{m_1 e^{i\xi_{\mathbf{m}} \cdot \mathbf{x}_0}}{(|\xi_{\mathbf{m}} + \mathbf{K}|^2 - \lambda')^2} \right|}{\sum_{\mathbf{m} \in \mathbb{Z}^2} \frac{1}{(|\xi_{\mathbf{m}} + \mathbf{K}|^2 - \lambda')^2}} \\ &= c(\lambda') \end{aligned}$$

This concludes that the directional derivative is independent of the direction  $\mathbf{u} \in \mathbb{S}^1$ .

We can show that  $\nabla_{\mathbf{u}} \lambda_-(\mathbf{K}) = -c(\lambda')$  by similar considerations.  $\square$

*Remark.* The coupling constant  $\alpha = (\alpha, \alpha)$  and the location of the point  $\mathbf{x}_0 = \frac{2}{3}(\mathbf{v}_1 + \mathbf{v}_2)$  in the fundamental domain  $\Gamma$  both play crucial roles in existence of conic singularities on dispersion surfaces since perturbed eigenvalues  $\lambda' \in \sigma(-\Delta_{\alpha, Y}(\mathbf{k})) \setminus \sigma(-\Delta(\mathbf{k}))$  of multiplicity 2 can only be obtained when the matrix  $\Gamma_{\alpha, \{0, \mathbf{x}_0\}}(\lambda, \mathbf{k})$  defined by (3.23) is a  $2 \times 2$  diagonal matrix with identical diagonal entries. In other words,  $\mathbf{x}_0$  determines if  $\Gamma_{\alpha, \{0, \mathbf{x}_0\}}(\lambda', \mathbf{k})$  is diagonal and  $\alpha = (\alpha, \alpha)$  makes those diagonal entries equal to each other so that the two dispersion surfaces meet at Dirac Point.

Now we observe two pairs of conic surfaces above and below the third dispersion surface, respectively.

**Theorem 4.9.** *Let  $\alpha \in \mathbb{R}$ . As  $\mathbf{k} \rightarrow \mathbf{K}$ ,*

$$\begin{aligned} \lambda_1(\mathbf{k}, \alpha) - \lambda_1(\mathbf{K}, \alpha) &= -c(\lambda_1(\mathbf{K}, \alpha)) |\mathbf{k} - \mathbf{K}| + o(|\mathbf{k} - \mathbf{K}|) \\ \lambda_2(\mathbf{k}, \alpha) - \lambda_1(\mathbf{K}, \alpha) &= c(\lambda_1(\mathbf{K}, \alpha)) |\mathbf{k} - \mathbf{K}| + o(|\mathbf{k} - \mathbf{K}|) \\ \lambda_4(\mathbf{k}, \alpha) - \lambda_4(\mathbf{K}, \alpha) &= -c(\lambda_4(\mathbf{K}, \alpha)) |\mathbf{k} - \mathbf{K}| + o(|\mathbf{k} - \mathbf{K}|) \\ \lambda_5(\mathbf{k}, \alpha) - \lambda_4(\mathbf{K}, \alpha) &= c(\lambda_4(\mathbf{K}, \alpha)) |\mathbf{k} - \mathbf{K}| + o(|\mathbf{k} - \mathbf{K}|) \end{aligned}$$

*Proof.* By Proposition 4.5,

$$\lambda_1^\infty(\mathbf{K}) = |\xi_{(0,0)} + \mathbf{K}| = |\xi_{(-1,-1)} + \mathbf{K}| = |\xi_{(-1,0)} + \mathbf{K}|$$

is an eigenvalue of  $-\Delta_{\alpha, \{0, \mathbf{x}_0\}}(\mathbf{K})$  of multiplicity 1. Then  $\lambda_3(\mathbf{K}, \alpha) = \lambda_1^\infty(\mathbf{K})$  since we obtain  $\lambda_1(\mathbf{K}, \alpha) = \lambda_2(\mathbf{K}, \alpha)$  and  $\lambda_4(\mathbf{K}, \alpha) = \lambda_5(\mathbf{K}, \alpha)$  by solving (4.3) on  $(-\infty, \lambda_1^\infty(\mathbf{K}))$  and  $(\lambda_1^\infty(\mathbf{K}), \lambda_2^\infty(\mathbf{K}))$ , respectively. Then we obtain the desired conclusion by applying Lemma 4.8 to  $\lambda_1(\mathbf{K}, \alpha) = \lambda_2(\mathbf{K}, \alpha)$  and  $\lambda_4(\mathbf{K}, \alpha) = \lambda_5(\mathbf{K}, \alpha)$ .  $\square$

*Remark.* Lemma 4.8 provides infinitely many pairs of 2-fold conic singularities at  $(\mathbf{K}, \lambda')$  where  $\lambda' \in \sigma(-\Delta_{\alpha, \{0, \mathbf{x}_0\}}(\mathbf{K})) \setminus \sigma(-\Delta(\mathbf{K}))$ . On the other hand, by Proposition 4.5, we observe a different kind of  $(3n-2)$ -fold conic singularities at  $(\mathbf{K}, \lambda')$  where  $\lambda' \in \sigma(-\Delta(\mathbf{K}))$  and  $n$  defined by (4.17) is greater than 1. For instance, the

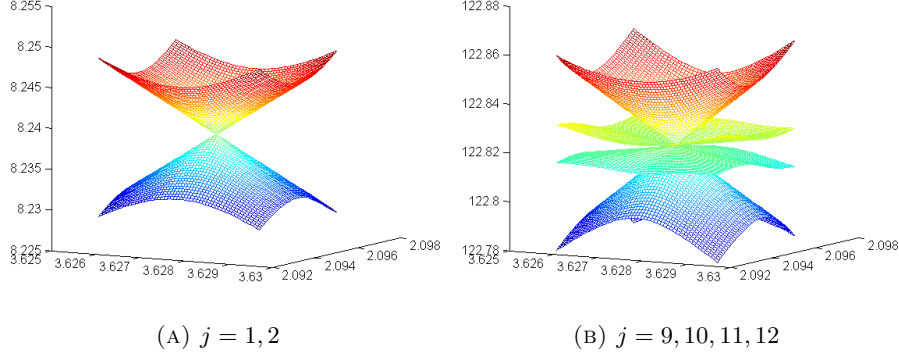


FIGURE 10. Local view of the  $j$ -th dispersion surfaces generated by  $-\Delta_{0,\{0,\mathbf{x}_0\}}(\mathbf{k})$  near Dirac Point  $\mathbf{K}$ . See <http://math.berkeley.edu/~lmj0425/floq2dual.avi> for the first five dispersion surfaces where  $\alpha$  varies from 100 to  $-100$ .

$j$ -th dispersion surfaces with  $j = 9, \dots, 12$  form a 4-fold conic singularity at Dirac point. See Figure 10 for both kinds of conic surfaces at Dirac point.

Due to the global asymptotic behavior of dispersion surfaces described in Theorem 4.6, the conic points also approach another surface as  $\alpha \rightarrow \pm\infty$ . In particular, as  $\alpha \rightarrow \infty$ ,

$$\lambda_1(\mathbf{K}, \alpha) = \lambda_2(\mathbf{K}, \alpha) \nearrow |\mathbf{K}^2|$$

where  $\lambda_3(\mathbf{K}, \alpha) = \lambda_1^\infty(\mathbf{K}) = |\mathbf{K}^2|$  is independent of  $\alpha$ . On the other hand, as  $\alpha \rightarrow -\infty$ ,

$$\lambda_1(\mathbf{K}, \alpha) = \lambda_2(\mathbf{K}, \alpha) \rightarrow -\infty$$

$$\lambda_4(\mathbf{K}, \alpha) = \lambda_5(\mathbf{K}, \alpha) \searrow |\mathbf{K}^2|.$$

**4.2.2. Spectral properties of the full Hamiltonian.** By Proposition 3.7, the full Hamiltonian of the honeycomb lattice point scatterer  $-\Delta_{\beta,H}$ ,  $\beta = (\alpha, \alpha, \dots)$  generates a spectrum given by the union of  $\sigma(-\Delta_{\alpha,\{0,\mathbf{x}_0\}}(\mathbf{k}))$  for all  $\mathbf{k} \in \mathcal{B}$ . Furthermore,  $\sigma(-\Delta_{\beta,H})$  formulates a band structure due to the continuity of each dispersion surface. More precisely, we obtain a union of infinitely many intervals induced by all dispersion surfaces:

$$(4.35) \quad \sigma(-\Delta_{\beta,H}) = \bigcup_{j \geq 1} \left[ \min_{\mathbf{k} \in \mathcal{B}} \lambda_j(\mathbf{k}, \alpha), \max_{\mathbf{k} \in \mathcal{B}} \lambda_j(\mathbf{k}, \alpha) \right].$$

Although a generic dispersion surface  $\mathbf{k} \mapsto \lambda_j(\mathbf{k}, \alpha)$  attains its maximum and minimum at various points  $\mathbf{k} \in \mathcal{B}$  that depends on  $\alpha$ , we observe a simple result at least for the lowest level.

**Proposition 4.10.** *For any  $\alpha \in (-\infty, \infty]$ , the lowest eigenvalue of the first band occurs at  $\mathbf{k} = \mathbf{0}$ , namely,*

$$\min_{\mathbf{k} \in \mathcal{B}} \lambda_1(\mathbf{k}, \alpha) = \lambda_1(\mathbf{0}, \alpha).$$

*Proof.* This can be proved easily when  $\alpha = \infty$  since

$$\lambda_1(\mathbf{k}, \infty) = \lambda_1^\infty(\mathbf{k}) = |\mathbf{k}|^2.$$

Now suppose  $\alpha \in \mathbb{R}$ . Then  $\lambda_1(\mathbf{k}, \alpha)$  is obtained by solving (4.19) on  $(-\infty, \lambda_1^\infty(\mathbf{k}))$  where the RHS of the equation is continuous and increasing as a function of  $\lambda$ . Since  $\lambda_1(\mathbf{k}, \alpha) < \lambda_1^\infty(\mathbf{k})$ , it suffices to show that

$$\alpha \geq g_{\lambda_1(\mathbf{0}, \alpha)}(\mathbf{0}, \mathbf{k}) + |g_{\lambda_1(\mathbf{0}, \alpha)}(\mathbf{x}_0, \mathbf{k})|$$

or equivalently,

$$g_{\lambda_1(\mathbf{0}, \alpha)}(\mathbf{0}, \mathbf{0}) + |g_{\lambda_1(\mathbf{0}, \alpha)}(\mathbf{x}_0, \mathbf{0})| \geq g_{\lambda_1(\mathbf{0}, \alpha)}(\mathbf{0}, \mathbf{k}) + |g_{\lambda_1(\mathbf{0}, \alpha)}(\mathbf{x}_0, \mathbf{k})|.$$

By Lemma 3.4, for  $\text{Im } \sqrt{\lambda} > 0$  and  $\mathbf{x} \in \Gamma$ ,

$$g_\lambda(\mathbf{x}, \mathbf{k}) = \begin{cases} \sum_{\mathbf{v} \in \Lambda} G_\lambda(\mathbf{x} + \mathbf{v}) e^{-i\mathbf{k} \cdot \mathbf{v}} & \text{if } \mathbf{x} \in \Gamma \setminus \{\mathbf{0}\} \\ \sum_{\substack{\mathbf{v} \in \Lambda \\ \mathbf{v} \neq \mathbf{0}}} G_\lambda(\mathbf{v}) e^{-i\mathbf{k} \cdot \mathbf{v}} + \frac{1}{2\pi} \ln \left( \frac{\sqrt{\lambda}}{i} \right) & \text{if } \mathbf{x} = \mathbf{0} \end{cases}$$

Since  $\lambda_1(\mathbf{0}, \alpha) < \lambda_1^\infty(\mathbf{0}) = 0$ , we have  $G_{\lambda_1(\mathbf{0}, \alpha)}(\mathbf{x}) > 0$  for  $\mathbf{x} \in \mathbb{R}^2 \setminus \{\mathbf{0}\}$ . So we obtain

$$\begin{aligned} & g_{\lambda_1(\mathbf{0}, \alpha)}(\mathbf{0}, \mathbf{k}) + |g_{\lambda_1(\mathbf{0}, \alpha)}(\mathbf{x}_0, \mathbf{k})| \\ &= \sum_{\substack{\mathbf{v} \in \Lambda \\ \mathbf{v} \neq \mathbf{0}}} G_{\lambda_1(\mathbf{0}, \alpha)}(\mathbf{v}) e^{-i\mathbf{k} \cdot \mathbf{v}} + \frac{1}{2\pi} \ln \left( \frac{\sqrt{\lambda_1(\mathbf{0}, \alpha)}}{i} \right) + \left| \sum_{\mathbf{v} \in \Lambda} G_{\lambda_1(\mathbf{0}, \alpha)}(\mathbf{x}_0 + \mathbf{v}) e^{-i\mathbf{k} \cdot \mathbf{v}} \right| \\ &\leq \sum_{\substack{\mathbf{v} \in \Lambda \\ \mathbf{v} \neq \mathbf{0}}} G_{\lambda_1(\mathbf{0}, \alpha)}(\mathbf{v}) + \frac{1}{2\pi} \ln \left( \frac{\sqrt{\lambda_1(\mathbf{0}, \alpha)}}{i} \right) + \left| \sum_{\mathbf{v} \in \Lambda} G_{\lambda_1(\mathbf{0}, \alpha)}(\mathbf{x}_0 + \mathbf{v}) \right| \\ &= g_{\lambda_1(\mathbf{0}, \alpha)}(\mathbf{0}, \mathbf{0}) + |g_{\lambda_1(\mathbf{0}, \alpha)}(\mathbf{x}_0, \mathbf{0})| \end{aligned}$$

which implies

$$\min_{\mathbf{k} \in \mathcal{B}} \lambda_1(\mathbf{k}, \alpha) = \lambda_1(\mathbf{0}, \alpha)$$

□

On the other hand, recall that the full Hamiltonian of a triangular lattice point scatterer has a spectrum consisting of at most two intervals by Proposition 4.2. We now observe an analogous result for honeycomb lattice point scatterers. See Figure 11 for the graph of spectral bands  $\sigma(-\Delta_{\beta, H})$  versus  $\alpha$  where  $\beta = (\alpha, \alpha, \dots)$ .

**Theorem 4.11.** *For  $\alpha \in \mathbb{R}$  and  $\beta = (\alpha, \alpha, \dots)$ , the spectrum of  $-\Delta_{\beta, H}$  consists of at most three disjoint intervals, namely,*

$$\sigma(-\Delta_{\beta, H}) = I_1 \cup I_2 \cup I_3$$

where

$$(4.36) \quad I_1 = \left[ \lambda_1(\mathbf{0}, \alpha), \max_{\mathbf{k} \in \mathcal{B}} \lambda_2(\mathbf{k}, \alpha) \right]$$

$$(4.37) \quad I_2 = \left[ \min_{\mathbf{k} \in \mathcal{B}} \lambda_3(\mathbf{k}, \alpha), \max_{\mathbf{k} \in \mathcal{B}} \lambda_3(\mathbf{k}, \alpha) \right]$$



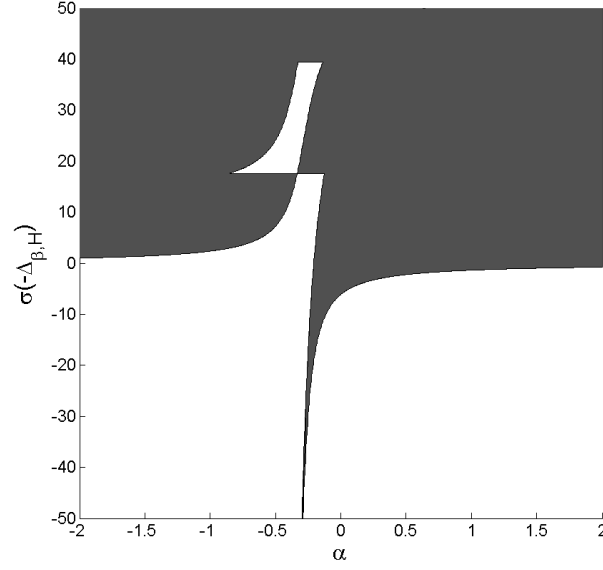


FIGURE 11. Spectrum of the honeycomb lattice point scatterer  $-\Delta_{\beta,H}$ ,  $\beta = (\alpha, \alpha, \dots)$  with respect to the coupling constant  $\alpha$ . The vertical section of the shaded region at each  $\alpha$  represents  $\sigma(-\Delta_{\beta,H})$

$$(4.38) \quad I_3 = \left[ \min_{\mathbf{k} \in \mathcal{B}} \lambda_4(\mathbf{k}, \alpha), \infty \right)$$

*Proof.* (4.37) is trivial due to the continuity of each dispersion surface  $\mathbf{k} \mapsto \lambda_j(\mathbf{k}, \alpha)$ . (4.36) can also be easily shown since we have

$$\min_{\mathbf{k} \in \mathcal{B}} \lambda_1(\mathbf{k}, \alpha) = \lambda_1(\mathbf{0}, \alpha)$$

and  $\lambda_1(\mathbf{K}, \alpha) = \lambda_2(\mathbf{K}, \alpha)$  by Proposition 4.10 and Proposition 4.7, respectively.

Now we prove all spectral bands except the first three levels consist of a single interval  $I_3$ . Fix  $\alpha \in \mathbb{R}$  and assume that there exists  $\tilde{\lambda} \notin \sigma(-\Delta_{\alpha, \{0, \mathbf{x}_0\}}(\mathbf{K}))$  such that

$$\tilde{\lambda} > \min_{\mathbf{k} \in \mathcal{B}} \lambda_4(\mathbf{k}, \alpha)$$

Then we can choose  $j' \geq 4$  such that

$$\lambda_{j'}(\mathbf{k}, \alpha) < \tilde{\lambda} < \lambda_{j'+1}(\mathbf{k}, \alpha), \quad \mathbf{k} \in \mathcal{B}$$

Also, it was proved by S.Albeverio [3] that

$$(4.39) \quad \lambda_{j-2}^\infty(\mathbf{k}) \leq \lambda_j(\mathbf{k}, \alpha) \leq \lambda_j^\infty(\mathbf{k}), \quad \mathbf{k} \in \mathcal{B}, \quad j \geq 3$$

where  $\lambda_j^\infty(\mathbf{k})$  is defined as in Theorem 4.6. So we have for all  $\mathbf{k} \in \mathcal{B}$ ,

$$(4.40) \quad \lambda_{j'-2}^\infty(\mathbf{k}) < \tilde{\lambda} < \lambda_{j'+1}^\infty(\mathbf{k}).$$

On the other hand, we know by the symmetry property of the dual lattice  $\Lambda^*$  that

$$(4.41) \quad \lambda_{6j+2}^\infty(\mathbf{0}) = \lambda_{6j+3}^\infty(\mathbf{0}) = \dots = \lambda_{6j+7}^\infty(\mathbf{0}), \quad j \geq 0$$

$$(4.42) \quad \lambda_{3j+1}^\infty(\mathbf{K}) = \lambda_{3j+2}^\infty(\mathbf{K}) = \lambda_{3j+3}^\infty(\mathbf{K}), \quad j \geq 0$$

By (4.40) and (4.41), we can choose  $j'' \geq 1$  such that

$$\lambda_{6j''+1}^\infty(\mathbf{0}) < \tilde{\lambda} < \lambda_{6j''+2}^\infty(\mathbf{0}).$$

Then by the assumption on  $\tilde{\lambda}$  and continuity of  $\mathbf{k} \mapsto \lambda_j^\infty(\mathbf{k})$ , we obtain

$$\lambda_{6j''+1}^\infty(\mathbf{K}) < \tilde{\lambda} < \lambda_{6j''+2}^\infty(\mathbf{K})$$

which contradicts (4.42). Hence,

$$\bigcup_{j \geq 4} \{\lambda_j(\mathbf{k}, \alpha) \mid \mathbf{k} \in \mathcal{B}\} = \left[ \min_{\mathbf{k} \in \mathcal{B}} \lambda_4(\mathbf{k}, \alpha), \infty \right)$$

□

#### ACKNOWLEDGEMENTS

The author is greatly indebted to Maciej Zworski for suggesting the topic as well as providing guidance throughout the research. The author was supported by the Samsung Scholarship.

#### REFERENCES

- [1] C. Fefferman, M. Weinstein, *Honeycomb Lattice Potentials and Dirac Points*, J. Amer. Math. Soc. 25 (2012), 1169-1220
- [2] S. Albeverio, F. Gesztesy, R. Høegh-Krohn, H. Holden, *Solvable Models in Quantum Mechanics* with an appendix by Pavel Exner. AMS Chelsea Publishing, 2nd Edition, (2005)
- [3] S. Albeverio, V.A. Geyler *The band structure of the general periodic Schrödinger operator with point interactions*. Commun. Math. Phys. 210 (2000), 29-48.
- [4] Z. Rudnick, H. Ueberschär, *Statistics of Wave Functions for a Point Scatterer on the Torus*. Commun. Math. Phys. 316, 763–782 (2012)
- [5] H. Ueberschär, *Quantum Chaos for Point Scatterers on Flat Tori*. preprint, arXiv:1212.1086
- [6] Y. Colin de Verdière, *Pseudo-laplaciens. I.. Annales de l'institut Fourier*, 32 no. 3 (1982), 275-286
- [7] A.H. Castro Neto, F. Guinea, N.M.R. Peres, K.S. Novoselov, A.K. Geim, *The electronic properties of graphene*. Rev. Mod. Phys., 81 (2009), 109–162
- [8] M. Reed, B. Simon, *Methods of Mathematical Physics II: Fourier Analysis, Self-Adjointness*. Academic Press, New York, (1975)
- [9] M. Reed, B. Simon, *Methods of Mathematical Physics IV: Analysis of Operators*. Academic Press, New York, (1978)
- [10] C. Kittel, *Introduction to Solid State Physics*. Wiley, 8th edition, (2005)
- [11] R.de L. Kronig, W.G. Penney, *Quantum Mechanics of Electrons in Crystal Lattices*. Proce. Royal Society of London. Series A, 130(814), 499–513 (1931)
- [12] P.R. Wallace, *The band theory of graphite*. Phys. Rev., 71 (1947), p.622
- [13] K.S. Novoselov, et al., *Electric Field Effect in Atomically Thin Carbon Films*. Science, 306 no. 5696 (2004), 666-669

*E-mail address:* lee.minjae@math.berkeley.edu

DEPARTMENT OF MATHEMATICS, UNIVERSITY OF CALIFORNIA, BERKELEY